=> d ibib abs hitstr 1

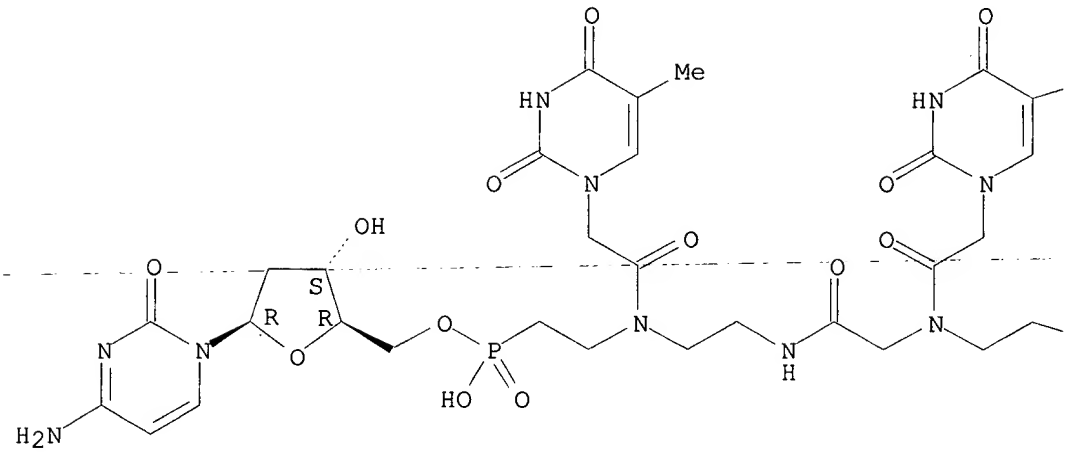
L13 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:893130 HCAPLUS
DOCUMENT NUMBER: 134:222969
TITLE: Synthesis and characterization of a tetranucleotide analog containing alternating phosphonate-amide backbone linkages
AUTHOR(S): Yu, P.; Wang, W.; Zhang, H.; Yang, X.; Liang, T. C.; Gao, X.
CORPORATE SOURCE: Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA
SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(1), 107-119
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:222969

AB Described herein is the synthesis and characterization of a tetranucleotide, 5'-dC-phosphonate-T-amide-T-phosphonate-dC (III), in which the C-T and T-C steps contain a phosphonate backbone bond and T-T is a peptide nucleic acid dimer unit (neutral backbone). The 5'- and 3'-OH groups of the tetramer can be further derivatized and, thus, the compd. is a potential building block for longer oligonucleotides which will contain alternating backbone modifications at designated positions. The synthesis involved first the prepn. of two hybrid peptide-deoxyribose dinucleotides, CT-CO (I) and N-CT (II) (C and T are nucleobases; CO and N are carboxylic and amino terminal, resp.); each is linked through a phosphonate linkage. A condensation reaction between the two dimers, followed by deprotection, resulted in the formation of a peptide linkage to give the desired tetramer III. The reaction conditions used are mild to afford products in moderate to excellent yields. The DNA-PNA-DNA tetramer, d(CTTC), is a substrate for T4 kinase but fails to give a ligation product, even though NMR shows weak interactions between the tetramer III with its complementary sequence, d(GAAG).

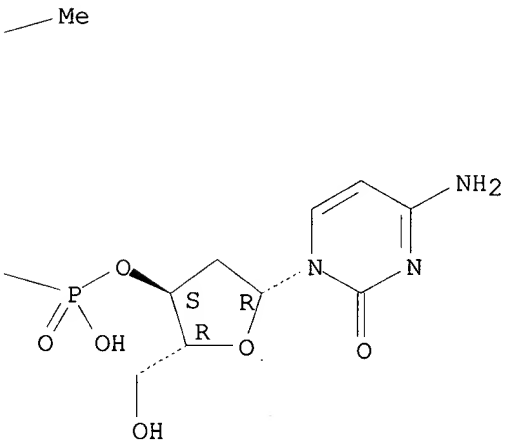
IT **329326-31-0P**
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(synthesis and characterization of a tetranucleotide analog contg. alternating phosphonate-amide backbone linkages as enzyme substrates)
RN 329326-31-0 HCAPLUS
CN Cytidine, 2'-deoxycytidylyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino](2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



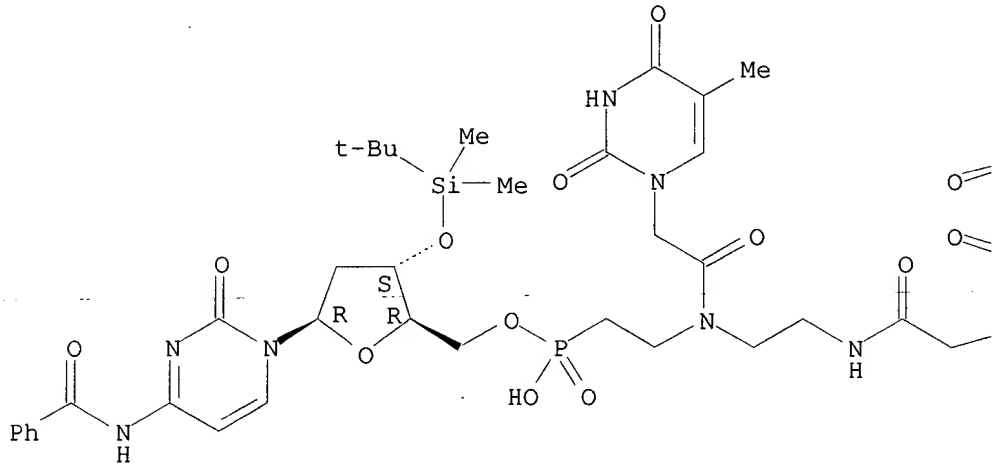
IT **329326-42-3P 329326-43-4P 329326-44-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and characterization of a tetranucleotide analog contg. alternating phosphonate-amide backbone linkages as enzyme substrates)

RN 329326-42-3 HCAPLUS

CN Cytidine, N-benzoyl-2'-deoxy-5'-O-[(1,1-dimethylethyl)dimethylsilyl]cytidyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino](2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-N-benzoyl-2'-deoxy-3'-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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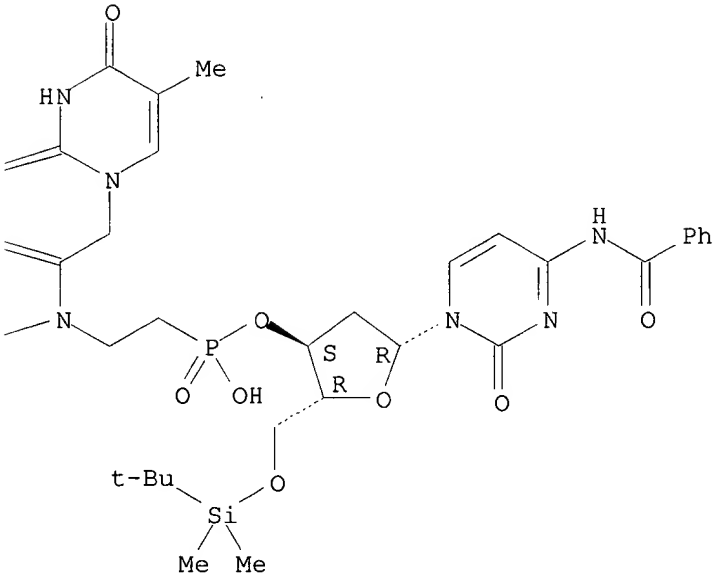
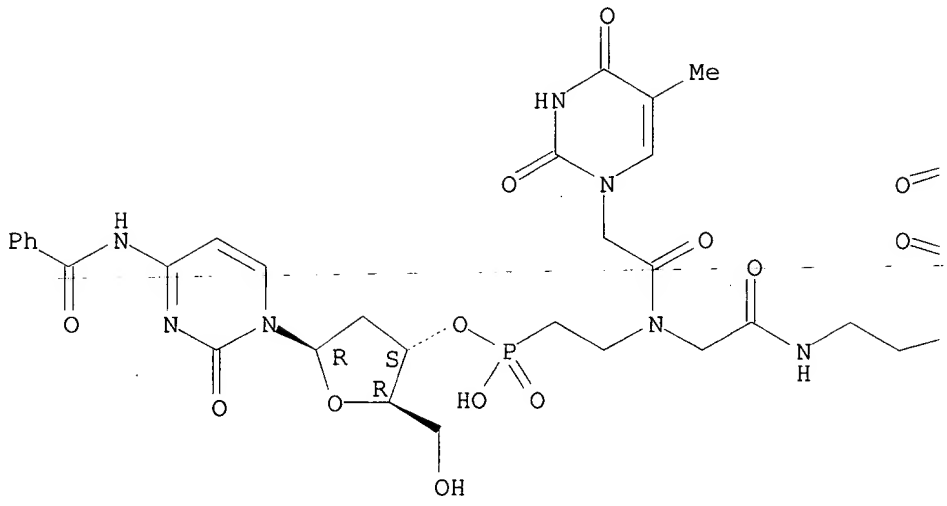


RN 329326-43-4 HCAPLUS
CN Cytidine, N-benzoyl-2'-deoxycytidylyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino](2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-N-benzoyl-2'-deoxy-3'-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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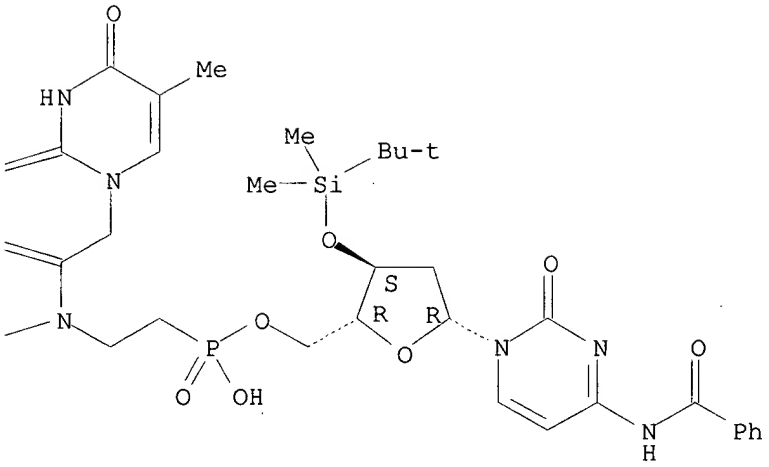
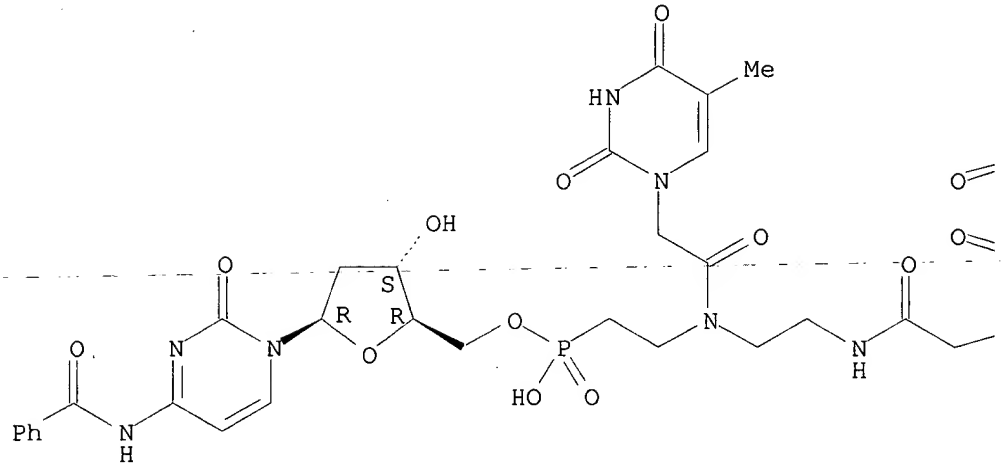


RN 329326-44-5 HCAPLUS
CN Cytidine, N-benzoyl-2'-deoxycytidylyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino](2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-N-benzoyl-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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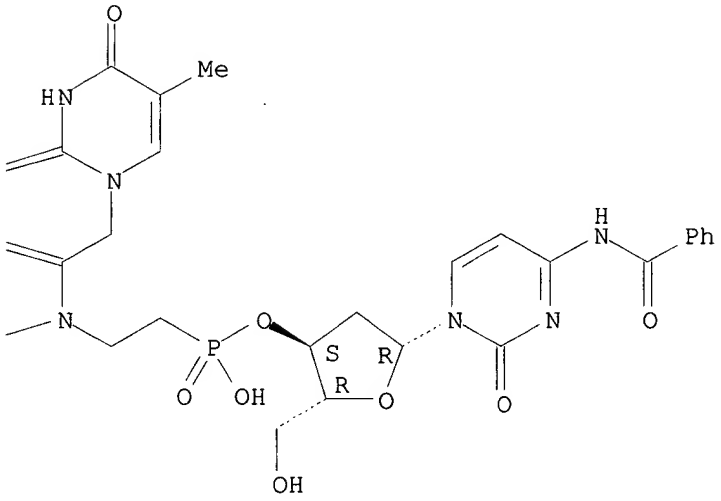

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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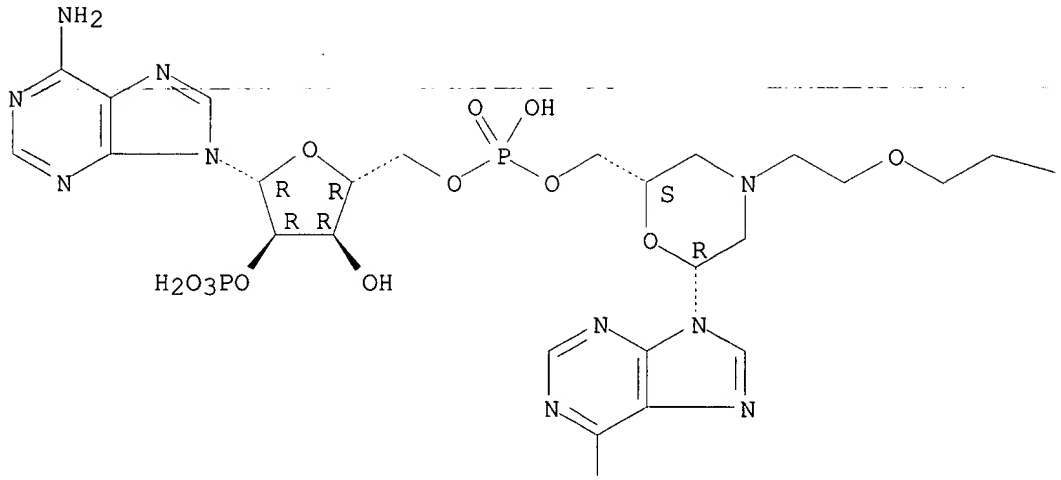
L13 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:458348 HCAPLUS
DOCUMENT NUMBER: 133:238287
TITLE: Convergent synthesis of ribonuclease L-active 2',5'-oligoadenylate-peptide nucleic acids
AUTHOR(S): Wang, Zhengfu; Chen, Ling; Bayly, Suzanne F.; Torrence, Paul F.
CORPORATE SOURCE: Section on Biomedical Chemistry, Laboratory of Medicinal Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0805, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2000), 10(12), 1357-1360
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 2-5A [(p5'A2')np5'A] was conjugated to N-(2-aminoethyl)-glycyl PNA by periodate oxidn., followed by coupling with amino-derivatized PNA and final cyanoborohydride redn. An adduct of 2-5A pentamer with tetrameric thymine PNA activated RNase L with the same potency as earlier versions of 2-5A-PNA or 2-5A-DNA.
IT **292609-04-2P 292609-05-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(convergent synthesis of RNase L-active oligoadenylate-peptide nucleic acids)
RN 292609-04-2 HCAPLUS
CN 2'-Adenylic acid, 5'-[[(2S,6R)-6-(6-amino-9H-purin-9-yl)-4-[41-amino-21,27,33,39-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8,17,23,29,35,41-hexaoxo-3,6,12,15-tetraoxa-9,18,21,24,27,30,33,36,39-nonaazahentetracont-1-yl]-2-morpholinyl]methyl hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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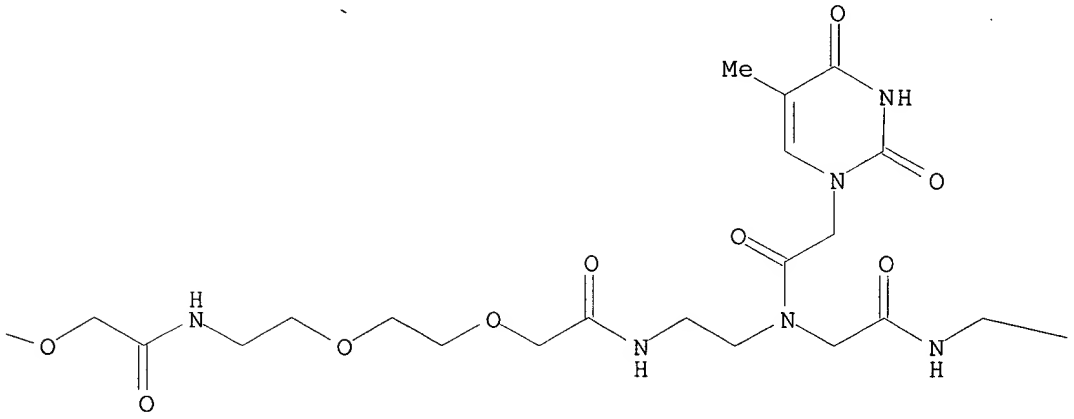

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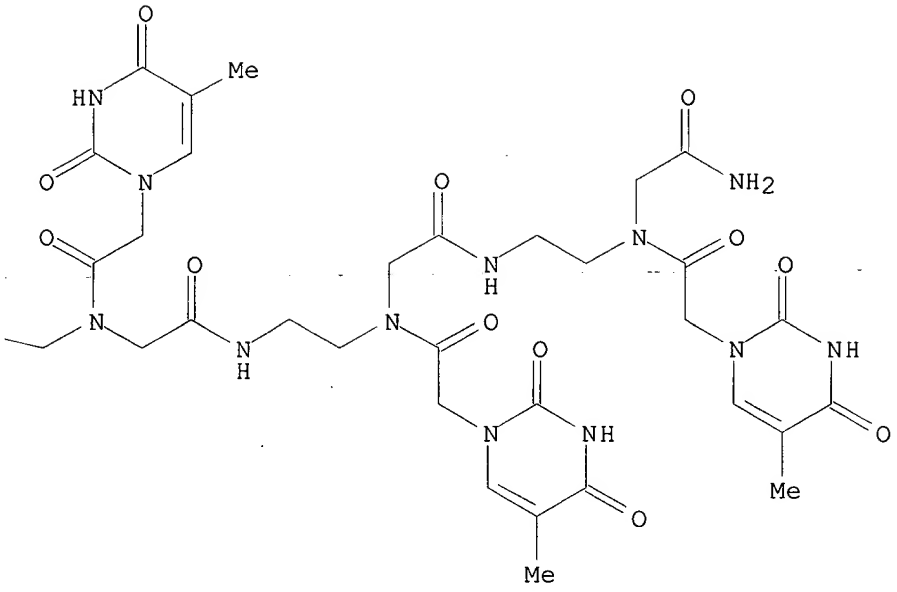
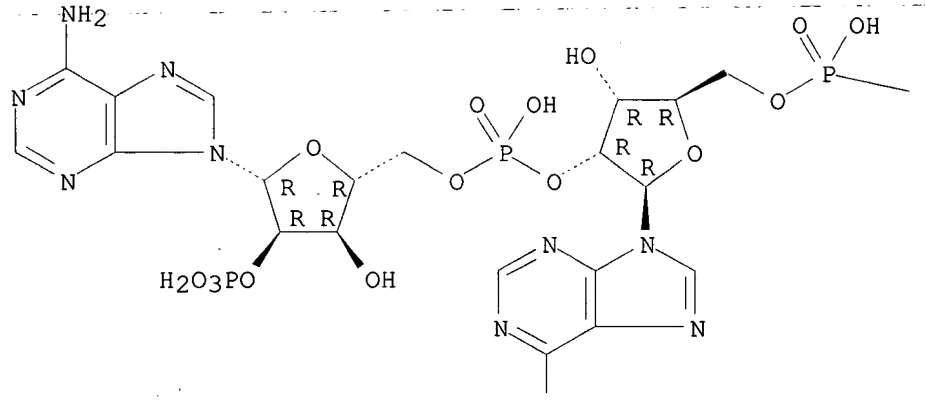


PAGE 2-A

RN 292609-05-3 HCAPLUS
CN 2'-Adenylic acid, 5'-O-[[[(2S,6R)-6-(6-amino-9H-purin-9-yl)-4-[41-amino-21,27,33,39-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8,17,23,29,35,41-hexaoxo-3,6,12,15-tetraoxa-9,18,21,24,27,30,33,36,39-nonaazahentetracont-1-yl]-2-morpholinyl]methoxy]hydroxyphosphinyl]adenylyl-(2'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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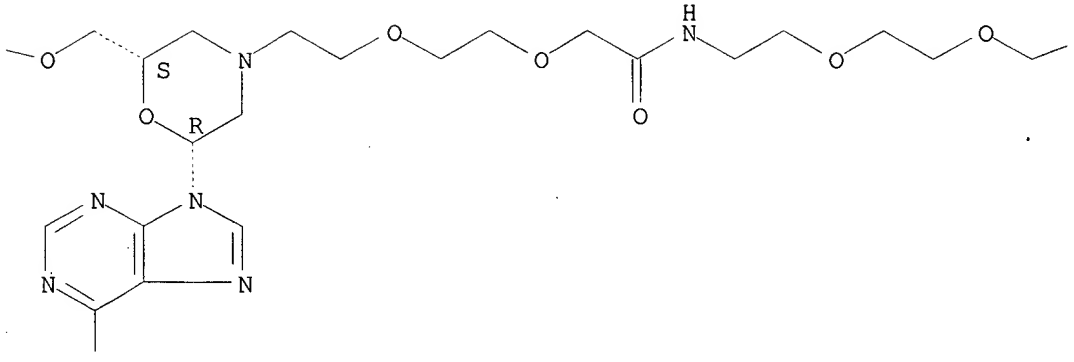

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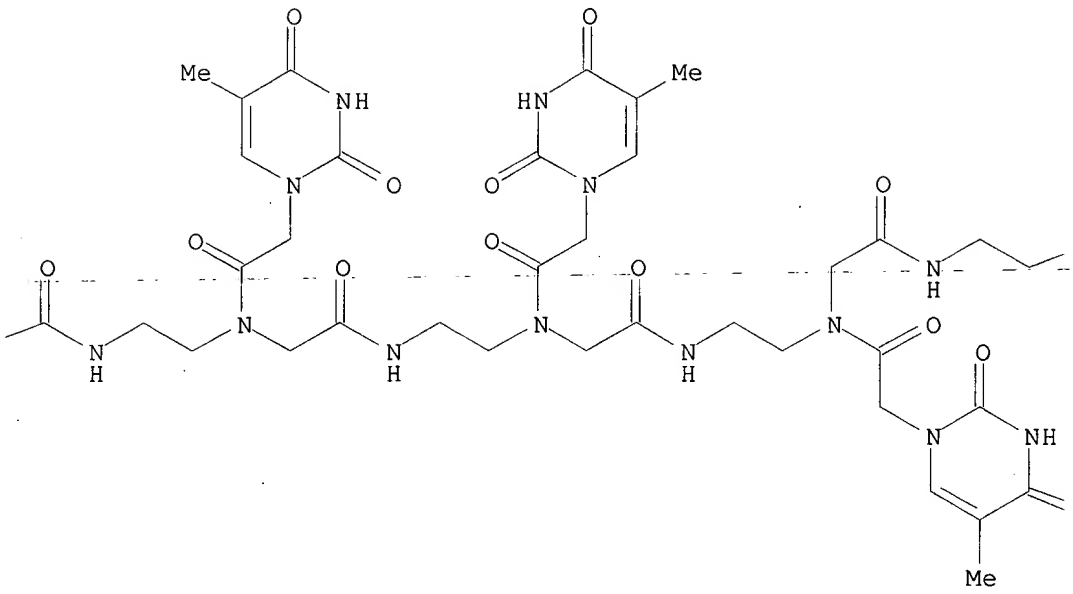

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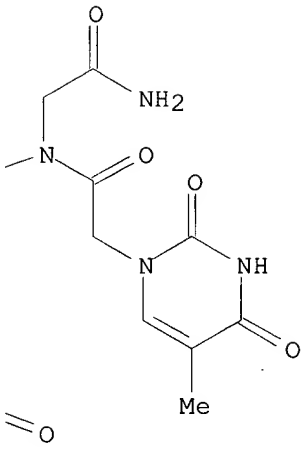


PAGE 2-A

NH_2

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 3

L13 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2000:89855 HCAPLUS
DOCUMENT NUMBER: 132:245836
TITLE: Acyclic Analogues of Deoxyadenosine 3',5'-Bisphosphates as P2Y1 Receptor Antagonists
AUTHOR(S): Kim, Yong-Chul; Gallo-Rodriguez, Carola; Jang, Soo-Yeon; Nandanan, Erathodiyil; Adams, Mary; Harden, T. Kendall; Boyer, Jose L.; Jacobson, Kenneth A.
CORPORATE SOURCE: Molecular Recognition Section Laboratory of Bioorganic Chemistry National Institute of Diabetes Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD, 20892-0810, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(4), 746-755
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

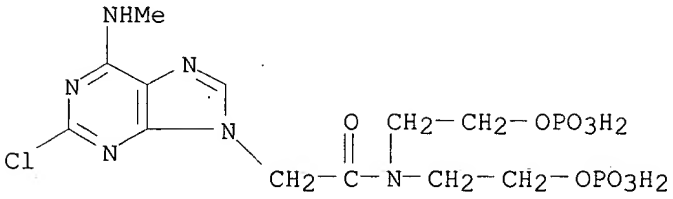
AB P2Y1 receptors are activated by ADP and occur on endothelial cells, smooth muscle, epithelial cells, lungs, pancreas, platelets, and in the central nervous system. With the aid of mol. modeling, we have designed nucleotide analogs that act as selective antagonists at this subtype. The present study has tested the hypothesis that acyclic modifications of the ribose ring, proven highly successful for nucleoside antiviral agents such as gancyclovir, are generalizable to P2Y receptor ligands. Specifically, the binding site of the P2Y1 receptor was found to be sufficiently accommodating to allow the substitution of the ribose group with acyclic aliph. and arom. chains attached to the 9-position of adenine. Three groups of adenine derivs. having diverse side-chain structures, each contg. two sym. phosphate or phosphonate groups, were prepd. Biol. activity was demonstrated by the ability of the acyclic derivs. to act as agonists or antagonists in the stimulation of phospholipase C in turkey erythrocyte membranes. An acyclic N6-methyladenine deriv., 2-[2-(6-methylamino-purin-9-yl)-ethyl]-propane-1,3-bisoxy(diammoniumphosphate) (10), contg. an isopentyl bisphosphate moiety, was a full antagonist at the P2Y1 receptor with an IC50 value of 1.60 .mu.M. The corresponding 2-Cl deriv. (11) was even more potent with an IC50 value of 0.84 .mu.M. Homologation of the ethylene group at the 9-position to 3-5 methylene units or inclusion of cis- or trans-olefinic groups greatly reduced antagonist potency at the P2Y1 receptor. Analogs contg. a diethanolamine amide group and an aryl di(methylphosphonate) were both less potent than 10 as antagonists, with IC50 values of 14 and 16 .mu.M, resp., and no agonist activity was obsd. for these analogs. Thus, the ribose moiety is clearly not essential for recognition by the turkey P2Y1 receptor, although a cyclic structure appears to be important for receptor activation, and the acyclic approach to the design of P2 receptor antagonists is valid.

IT **262863-42-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(acyclic analogs of deoxyadenosine 3',5'-bisphosphates as P2Y1 receptor antagonists)

RN 262863-42-3 HCAPLUS
CN 9H-Purine-9-acetamide, 2-chloro-6-(methylamino)-N,N-bis[2-(phosphonooxy)ethyl]-, compd. with N,N-diethylethanamine (1:1), triammonium salt (9CI) (CA INDEX NAME)

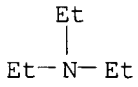
CM 1

CRN 262863-41-2
CMF C12 H19 Cl N6 O9 P2

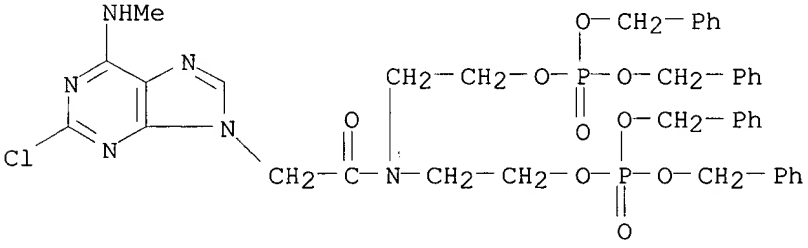


CM 2

CRN 121-44-8
CMF C6 H15 N



IT **262863-49-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(acyclic analogs of deoxyadenosine 3',5'-bisphosphates as P2Y1 receptor antagonists)
RN 262863-49-0 HCAPLUS
CN Phosphoric acid, [[[2-chloro-6-(methylamino)-9H-purin-9-yl]acetyl]imino]di-2,1-ethanediyl tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)



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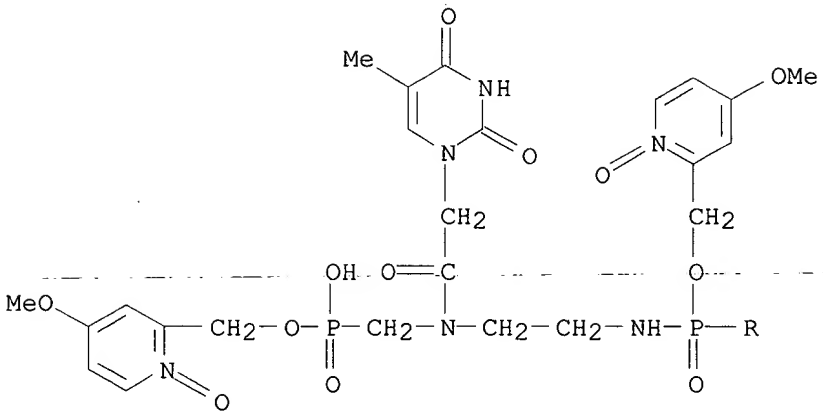
L13 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:290595 HCAPLUS
DOCUMENT NUMBER: 131:59111
TITLE: Peptide nucleic acids and their phosphonate analogues: synthesis and hybridization properties
AUTHOR(S): Efimov, V. A.; Buryakova, A. A.; Choob, M. V.; Chakhmakhlcheva, G.
CORPORATE SOURCE: Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow, 117871, Russia
SOURCE: Bioorganicheskaya Khimiya (1998), 24(9), 696-709
CODEN: BIKHD7; ISSN: 0132-3423
PUBLISHER: MAIK Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The synthesis of a series of DNA mimics (peptide nucleic acids, phosphonate analogs of peptide nucleic acids, and their hybrids) is described. The preparative synthesis of the corresponding monomers and the solid phase automated synthesis of oligomers-mimics are developed. Modified phosphonate analogs of peptide nucleic acids, in particular chiral derivs. and those with addnl. hydroxyl groups in the side chains of the backbone as well as pyrene derivs. of peptide nucleic acids and their phosphonate analogs, are prepd. The ability of the resulting oligomers specifically to hybridize to DNA and RNA complementary chains is studied. It is shown that phosphonate analogs of peptide nucleic acids and their hybrids with peptide nucleic acids can form complexes with the DNA and RNA complementary strands, the stability of the complexes increasing in parallel with the increase in the no. of peptide nucleic acid residues in the chain of the mimic. This property, along with good water soly., provides the precondition for further evaluation of these compds. as antisense and antigene agents.

IT **227798-10-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and hybridization properties of peptide nucleic acids and their phosphonate analogs)
RN 227798-10-9 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6-[(4-methoxy-1-oxido-2-pyridinyl)methoxy]-12-(4-methoxyphenyl)-6-oxido-12,12-diphenyl-2,5,8,11-tetraaza-6-phosphadodec-1-yl]-, mono[(4-methoxy-1-oxido-2-pyridinyl)methyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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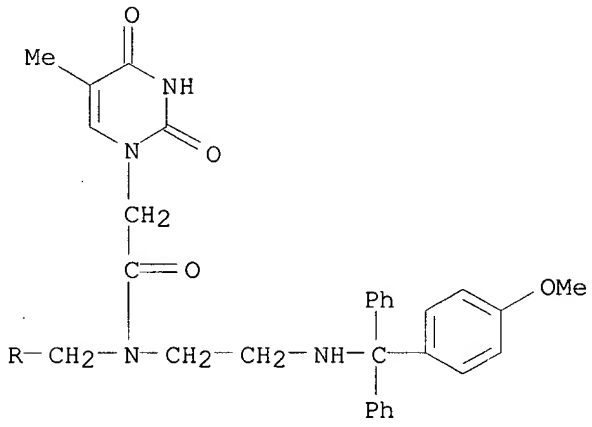

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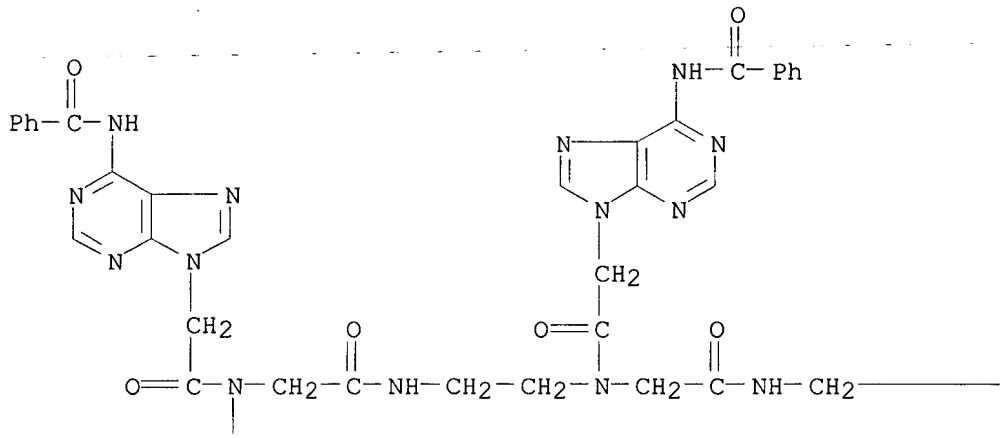
L13 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:235768 HCAPLUS
DOCUMENT NUMBER: 131:19274
TITLE: 2',5'-oligoadenylate-peptide nucleic acids (2-5A-PNAs) activate RNase L
AUTHOR(S): Verheijen, Jeroen C.; Van der Marel, Gijsbert A.; Van Boom, Jacques H.; Bayly, Suzanne F.; Player, Mark R.; Torrence, Paul F.
CORPORATE SOURCE: Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.
SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(3), 449-455
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB To potentiate the 2-5A (2',5'-oligoadenylate)-antisense and peptide nucleic acid (PNA) approaches to regulation of gene expression, composite mols. were generated contg. both 2-5A and PNA moieties. 2-5A-PNA adducts were synthesized using solid-phase techniques. Highly cross-linked polystyrene beads were functionalized with glycine tethered through a p-hydroxymethyl-benzoic acid linker and the PNA domain of the chimeric oligonucleotide analog was added by sequential elongation of the amino terminus with the monomethoxytrityl protected N-(2-aminoethyl)-N-(adenin-1-ylacetyl)glycinate. Transition to the 2-5A domain was accomplished by coupling of the PNA chain to dimethoxytrityl protected N-(2-hydroxyethyl)-N-(adenin-1-ylacetyl)glycinate. Finally, (2-cyanoethyl)-N,N-diisopropyl-4-O-(4,4-dimethoxytrityl)butyl-phosphoramidite and the corresponding (2-cyanoethyl)-N,N-diisopropylphosphoramidite of 5-O-(4,4'-dimethoxytrityl)-3-O-(tert-butyldimethylsilyl)-N6-benzoyl-adenosine were the synthons employed to add the 2 butanediol phosphate linkers and the four 2',5'-linked riboadenylates. The 5'-phosphate moiety was introduced with 2-[[2-(4,4'-dimethoxytrityloxy)ethyl]sulfonyl]ethyl-(2-cyanoethyl)-N,N-diisopropylphosphoramidite. Deprotection with methanolic NH3 and tetraethylammonium fluoride afforded the desired products, 2-5A-pnaA4, 2-5A-pnaA8 and 2-5A-pnaA12. When evaluated for their ability to cause the degrdn. of two different RNA substrates by the 2-5A-dependent RNase L, these new 2-5A-PNA conjugates were found to be potent RNase L activators. The union of 2-5A and PNA presents fresh opportunities to explore the biol. and therapeutic implications of these unique approaches to antisense.
IT **225787-02-0DP**, solid-supported
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of in the synthesis of 2',5'-oligoadenylate-peptide nucleic acids (2-5A-PNAs) for activation of RNase L)
RN 225787-02-0 HCAPLUS
CN Peptide nucleic acid, ((deamino)(hydroxy)T-bz6A-bz6A-bz6A-bz6A)-Gly-OH, (4-carboxyphenyl)methyl ester, 5'-[2-cyanoethyl 4-[[(2-cyanoethoxy)(4-hydroxybutoxy)phosphinyl]oxy]butyl phosphate] (9CI) (CA INDEX NAME)

PAGE 1-A



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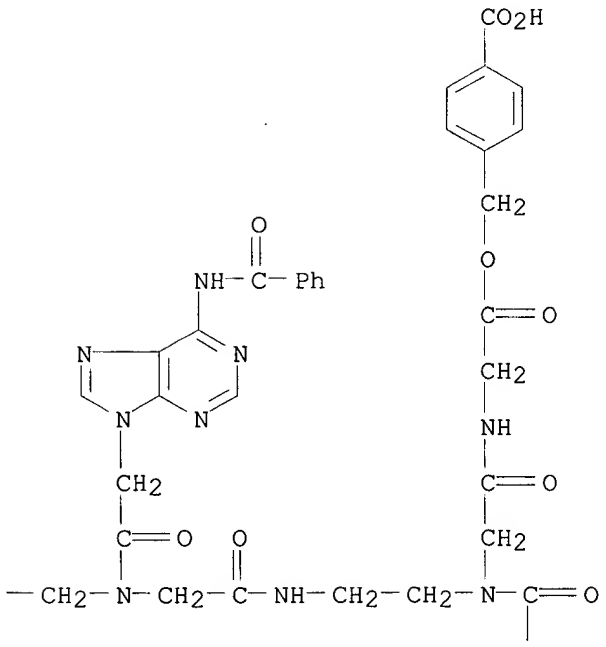
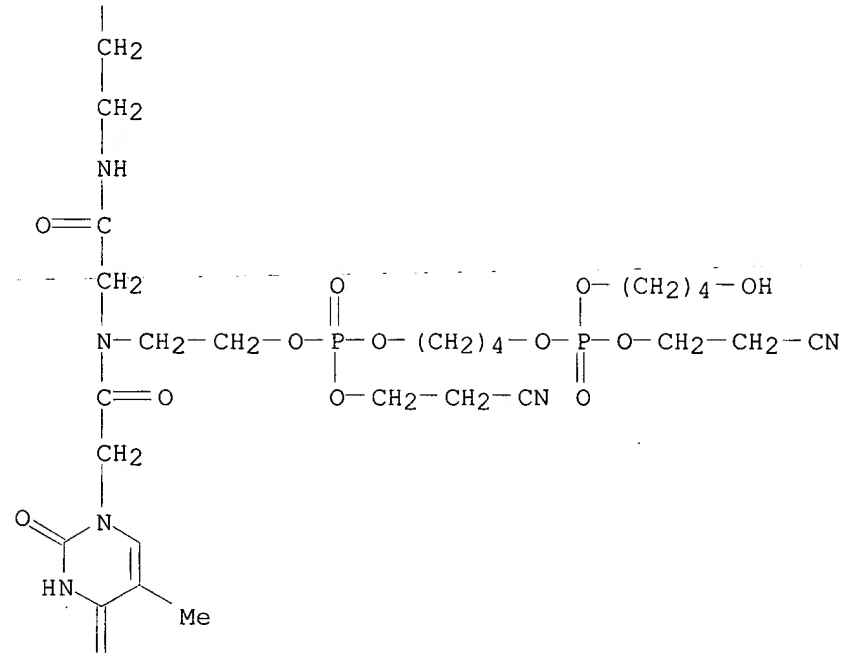
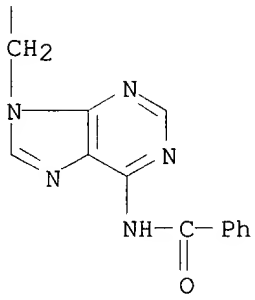


PAGE 2-A



PAGE 2-B



PAGE 3-A

REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

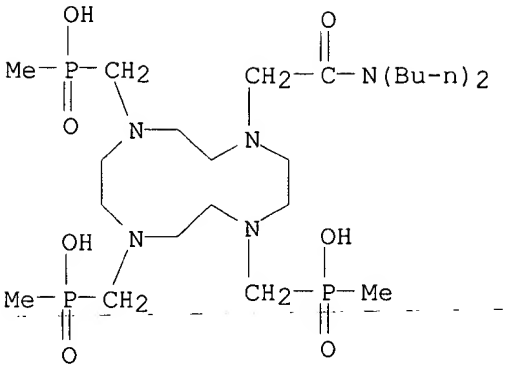
=> d ibib abs hitstr 6

L13 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1999:136456 HCAPLUS
DOCUMENT NUMBER: 130:357726
TITLE: Non-radiative deactivation of the excited states of europium, terbium and ytterbium complexes by proximate energy-matched OH, NH and CH oscillators: an improved luminescence method for establishing solution hydration states
AUTHOR(S): Beeby, Andrew; Clarkson, Ian M.; Dickins, Rachel S.; Faulkner, Stephen; Parker, David; Royle, Louise; de Sousa, Alvaro S.; Williams, J. A. Gareth; Woods, Mark
CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1999), (3), 493-504
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The radiative rate consts. for depopulation of the excited states of closely-related series of anionic, neutral and cationic Eu, Tb and Yb complexes were measured in H2O and D2O. With the aid of selective ligand deuteration, the relative contributions of OH, NH (both amide and amine) and CH oscillators were measured and critically assessed. Quenching of the Eu 5D0 excited state by amine NH oscillators is more than twice as efficient as OH quenching. The importance of the distance between the excited Ln ion and the XH oscillator is described with recourse to published crystallog. information. The general equation, q = A'(.DELTA.kH2O-kD2O)corr is presented and revised values of A' for Eu (1.2 ms), Tb (5 ms) and Yb (1 .mu.s) given, which allow for the quenching contribution of closely diffusing OH oscillators. The relevance of such studies to the hydration state of certain Gd complexes is described and clear evidence provided for a break in hydration at Gd.

IT **145130-40-1**
RL: PRP (Properties)
(complexes of Eu, Tb, Yb; non-radiative deactivation of excited states of europium, terbium and ytterbium complexes by proximate energy-matched OH, NH and CH oscillators: improved luminescence method for establishing soln. hydration states)

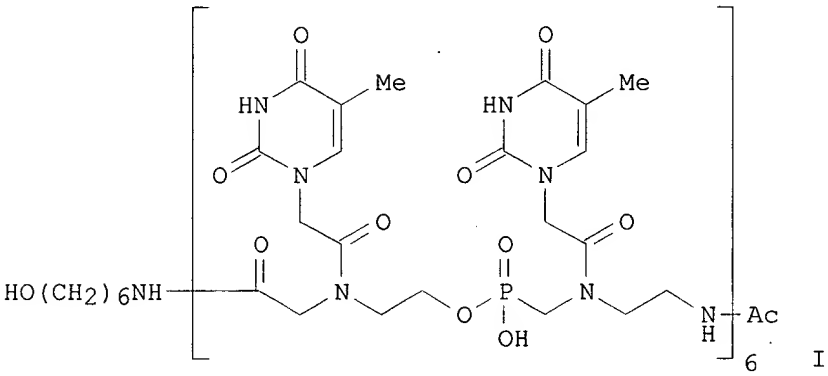
RN 145130-40-1 HCAPLUS
CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 7

L13 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1998:70167 HCAPLUS
DOCUMENT NUMBER: 128:167687
TITLE: PHONA - PNA co-oligomers: nucleic acid mimetics with interesting properties
AUTHOR(S): Peyman, Anusch; Uhlmann, Eugen; Wagner, Konrad; Augustin, Sascha; Weiser, Caroline; Will, David W.; Breipohl, Gerhard
CORPORATE SOURCE: Hoechst Marion Roussel Deutschland GmbH, Frankfurt, D-65926, Germany
SOURCE: Angewandte Chemie, International Edition in English (1998), Volume Date 1997, 36(24), 2809-2812
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

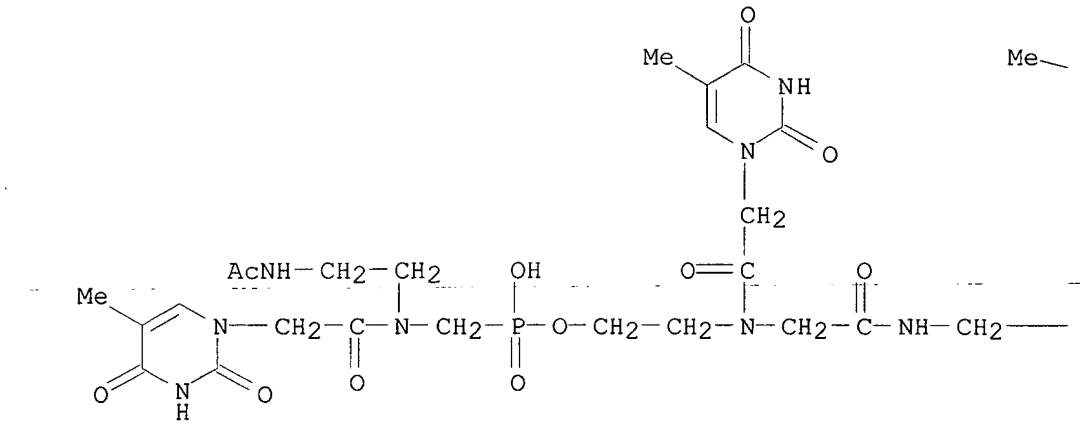
AB Alternating title co-oligomer I contg. peptide nucleic acid (PNA) and (aminomethyl)phosphonic acid backbones was prepd. and melting temps. (Tm) of complexes with completely or partially complementary DNA measured. The binding properties of I with complementary DNA are very similar to those of PNAs, but the co-oligomer I has a much better water soly.

IT **202914-68-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of (aminomethyl)phosphonic acid backbone peptide nucleic acid co-oligomers as nucleic acid mimetics with interesting properties)

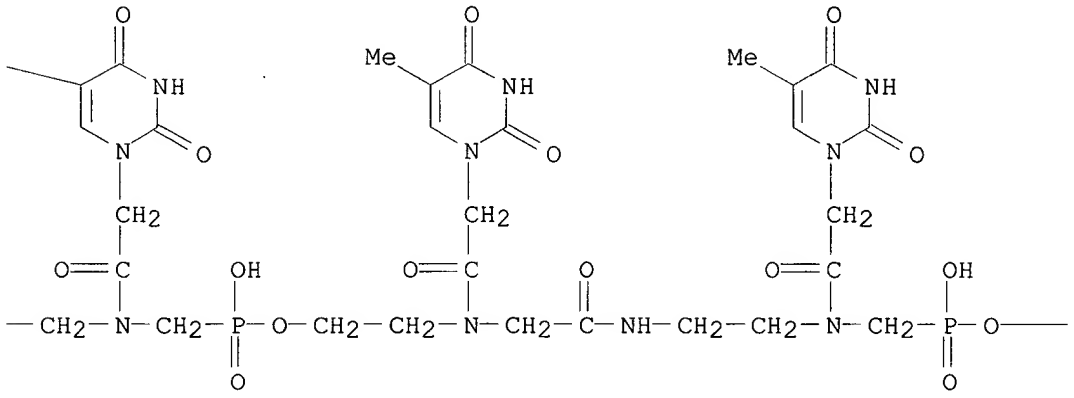
RN 202914-68-9 HCAPLUS

CN Phosphonic acid, [2,8,14,20,26,31,37-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12,24,35-trihydroxy-12,24,35-trioxido-6,18,30,41-tetraoxo-11,23,34-trioxa-2,5,8,14,17,20,26,29,31,37,40-undecaaza-12,24,35-triphosphadotetracont-1-yl]-, mono[3,9,15,21,27-pentakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11,23,36-trihydroxy-11,23-dioxido-5,17,29-trioxo-12,24-dioxa-3,6,9,15,18,21,27,30-octaaza-11,23-diphosphahexatriacont-1-yl] ester (9CI) (CA INDEX NAME)

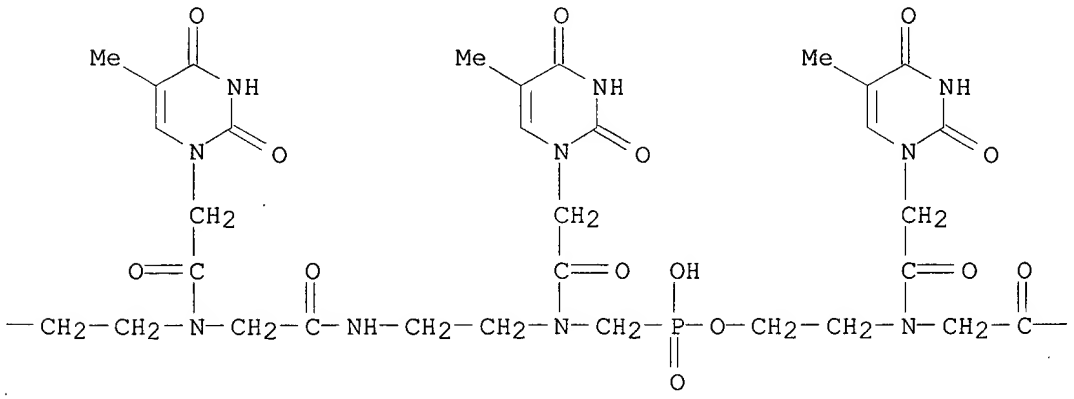
PAGE 1-A



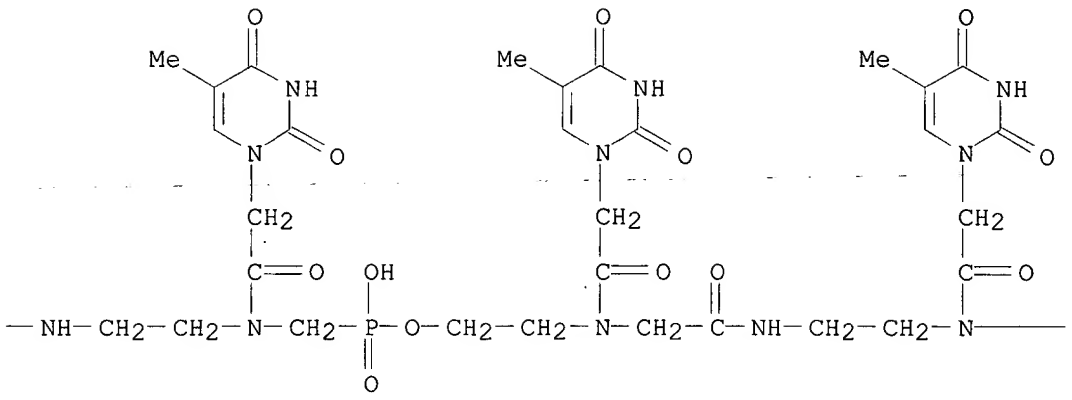
PAGE 1-B



PAGE 1-C



PAGE 1-D



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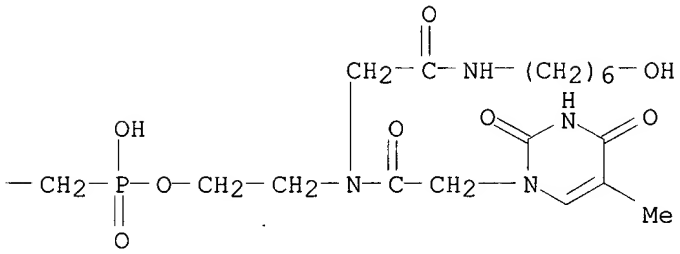


=> d ibib abs hitstr 8

L13 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1997:88503 HCAPLUS
DOCUMENT NUMBER: 126:100903
TITLE: Phosphonomonoester nucleic acids, process for their preparation, and their use in molecular biology and as pharmaceuticals
INVENTOR(S): Peyman, Anuschirwan; Uhlmann, Eugen; Breipohl, Gerhard; Wallmeier, Holger
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Can. Pat. Appl., 126 pp.
CODEN: CPXXEB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2171589	AA	19960914	CA 1996-2171589	19960312
DE 19508923	A1	19960919	DE 1995-19508923	19950313
DE 19543865	A1	19970605	DE 1995-19543865	19951124

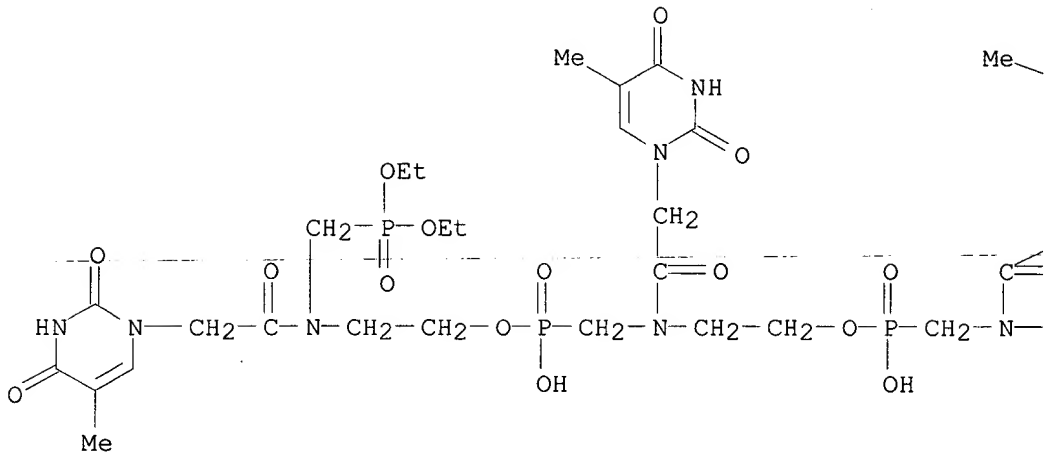
PRIORITY APPLN. INFO.: DE 1995-19508923 A 19950313
DE 1995-19543865 A 19951124
OTHER SOURCE(S): CASREACT 126:100903

AB Novel oligonucleotide analogs which may be loosely described as phosphonomonoester analogs of peptide nucleic acids (PMENA's) and methods for their synthesis are claimed. Particularly preferred PMENA analogs are Q-[OP(:O)(OR)CH2N(COCH2B)CH2CH2]nO-Q' (n=1-25; R=OH, OEt, OPh, etc.; B=natural nucleobase; Q,Q'=H, alkyl, Ph, etc. or an oligonucleotide or modified oligonucleotide). Their application relates to use as inhibitors of gene expression (antisense oligonucleotides, ribozymes, sense oligonucleotides and triplex-forming oligonucleotides), as probes for the detection of nucleic acids and as auxiliaries in mol. biol. PMENA analog H-[OP(:O)(OH)CH2N(COCH2T)CH2CH2]9OP(:O)(OEt)OEt was prepd. and its interaction with (dA)9 examd. by UV spectroscopy and by gel shift anal. The Tm for the PMENA analog-(dA)9 complex was 23.degree..

IT **185670-74-0P**
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(phosphonomonoester nucleic acids prepn. and use in mol. biol. and as pharmaceuticals)

RN 185670-74-0 HCAPLUS
CN Phosphonic acid, [28-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12,18,24-tetrahydroxy-26-(2-hydroxyethyl)-6,12,18,24-tetraoxido-27-oxo-5,11,17,23-tetraoxa-2,8,14,20,26-pentaaza-6,12,18,24-tetraphosphaoctacos-1-yl]-, mono[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-23-ethoxy-5,11,17-trihydroxy-5,11,17,23-tetraoxido-6,12,18,24-tetraoxa-3,9,15,21-tetraaza-5,11,17,23-tetraphosphahexacos-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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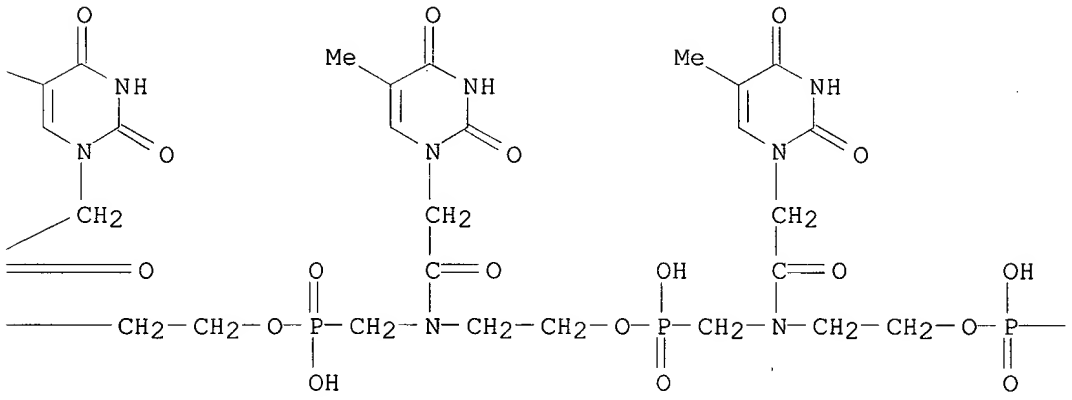

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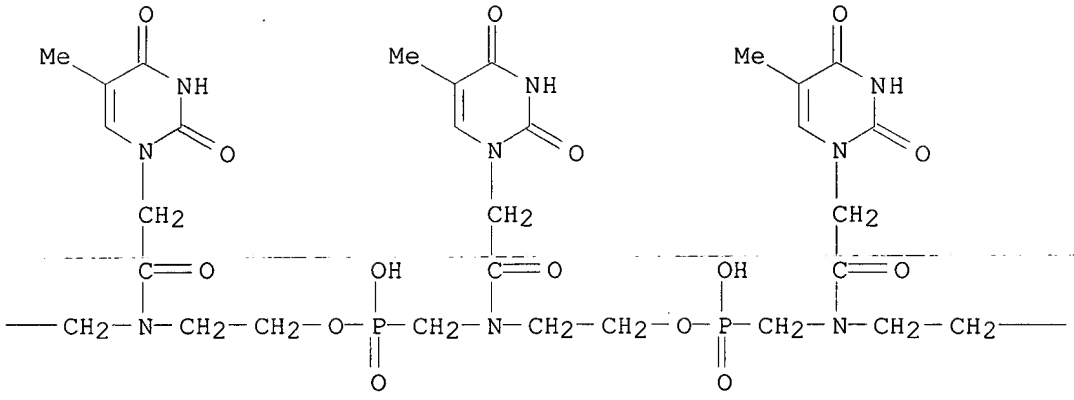

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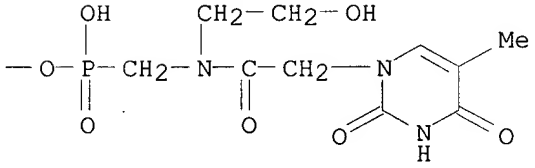
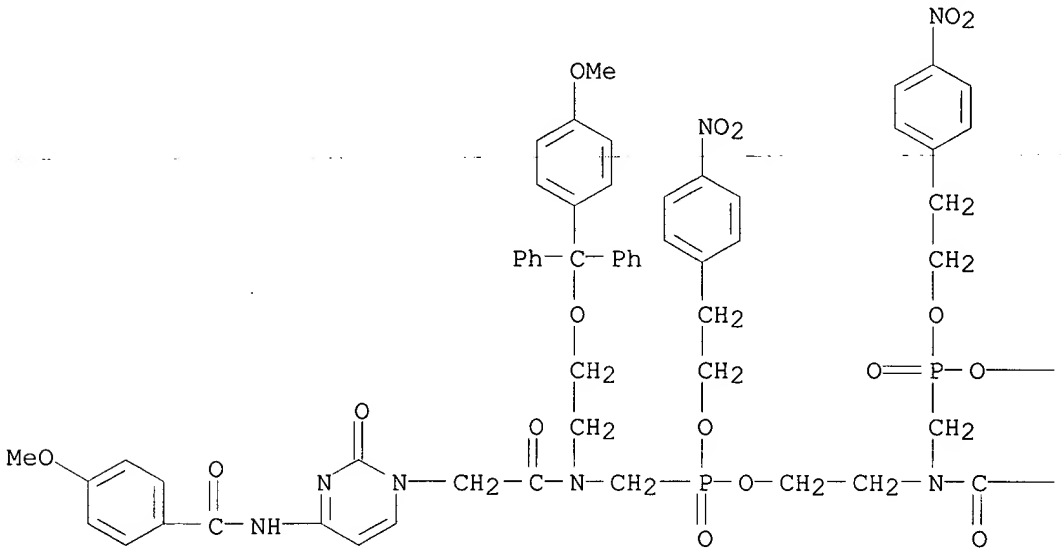


IT **183057-63-8P 183057-66-1P 183057-94-5P**
183057-96-7P 183057-99-0P 183058-04-0P
183058-06-2P 183058-09-5P 183058-10-8P
183058-11-9P 183058-12-0P 183058-13-1P
183058-14-2P 183058-15-3P 183058-16-4P
183058-18-6P 185670-60-4P 185670-61-5P
185670-62-6P 185670-63-7P 185670-64-8P
185670-65-9P 185670-66-0P 185670-67-1P
185670-68-2P 185670-69-3P 185670-70-6P
185670-71-7P 185670-72-8P 185670-95-5P
185670-96-6P 185670-97-7P 185670-98-8P
185670-99-9P 185671-00-5P 185671-01-6P
185671-02-7P 185671-03-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(phosphonomonoester nucleic acids prepn. and use in mol. biol. and as pharmaceuticals)
RN 183057-63-8 HCAPLUS
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-

pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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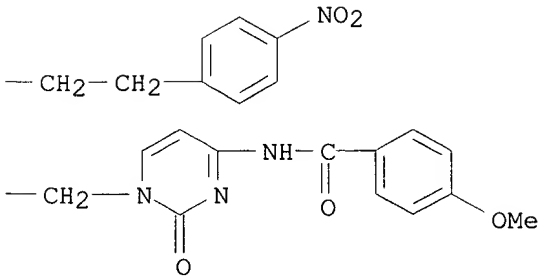
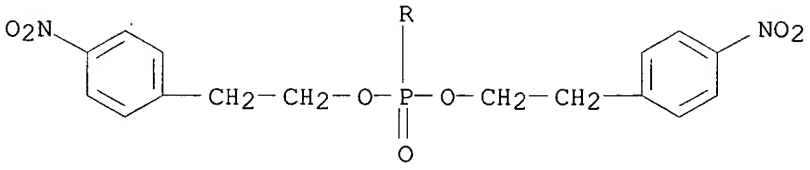
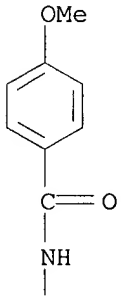


RN 183057-66-1 HCAPLUS

CN Phosphonic acid, [[(2-hydroxyethyl)[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]methyl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A





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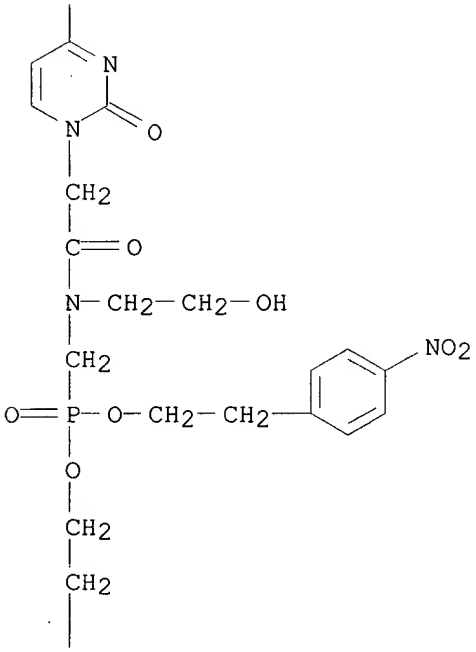
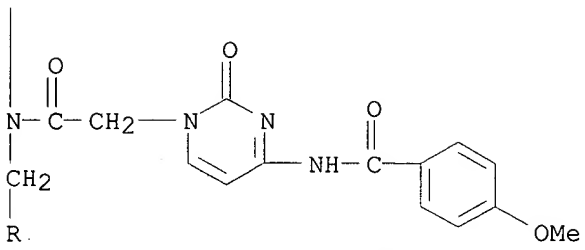
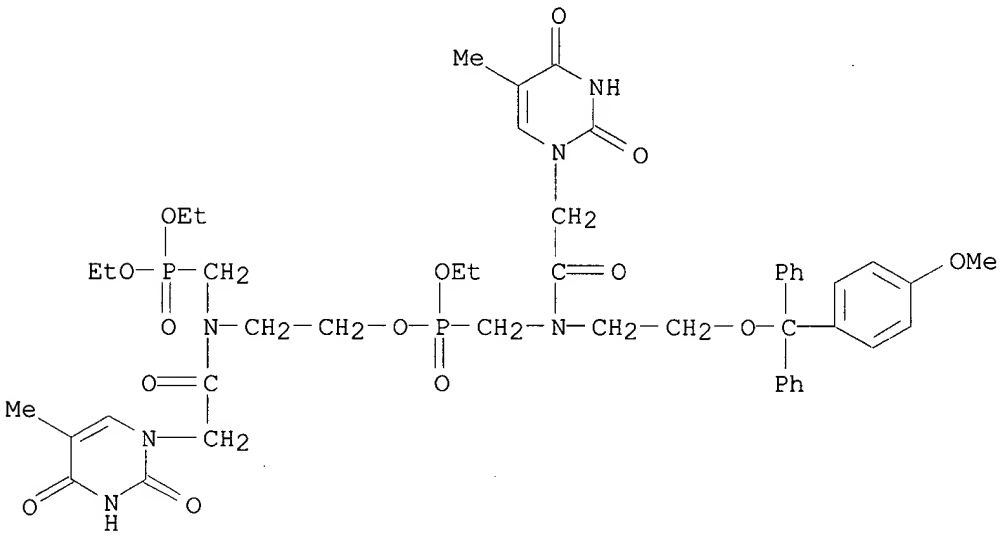


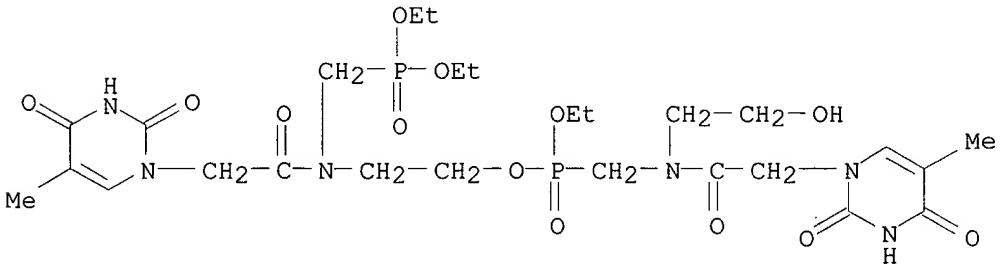
PAGE 3-A



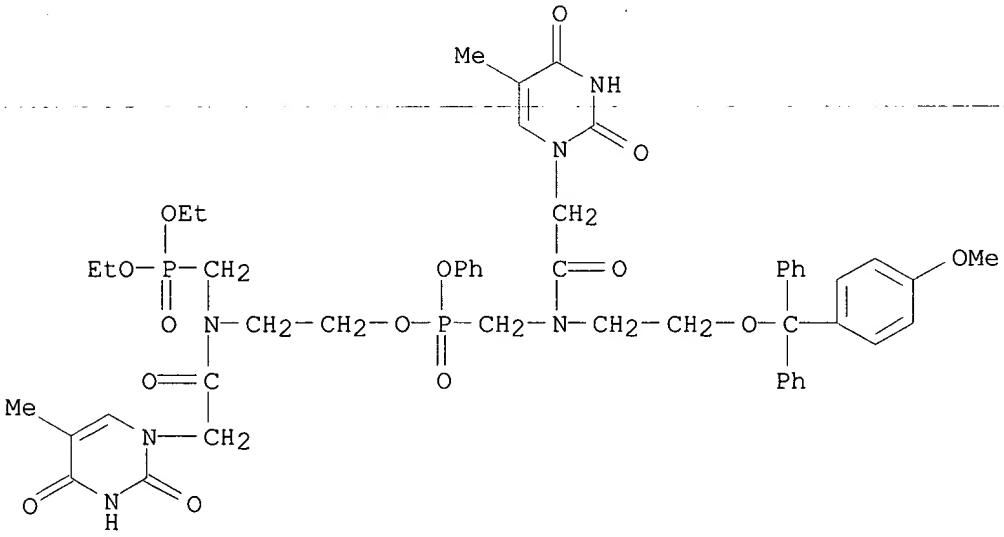
RN 183057-94-5 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6-ethoxy-12-(4-methoxyphenyl)-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 183057-96-7 HCAPLUS
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl ethyl ester (9CI) (CA INDEX NAME)



RN 183057-99-0 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-oxido-6-phenoxy-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 183058-04-0 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)

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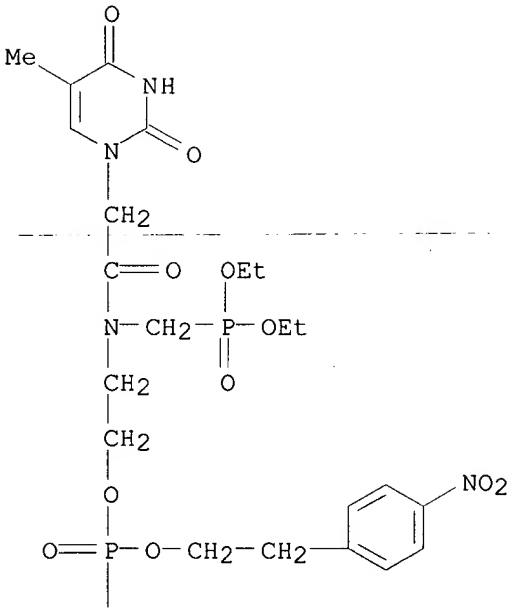

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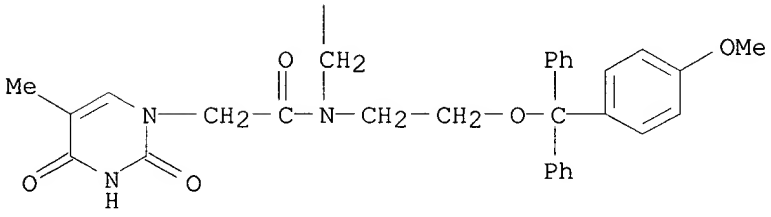
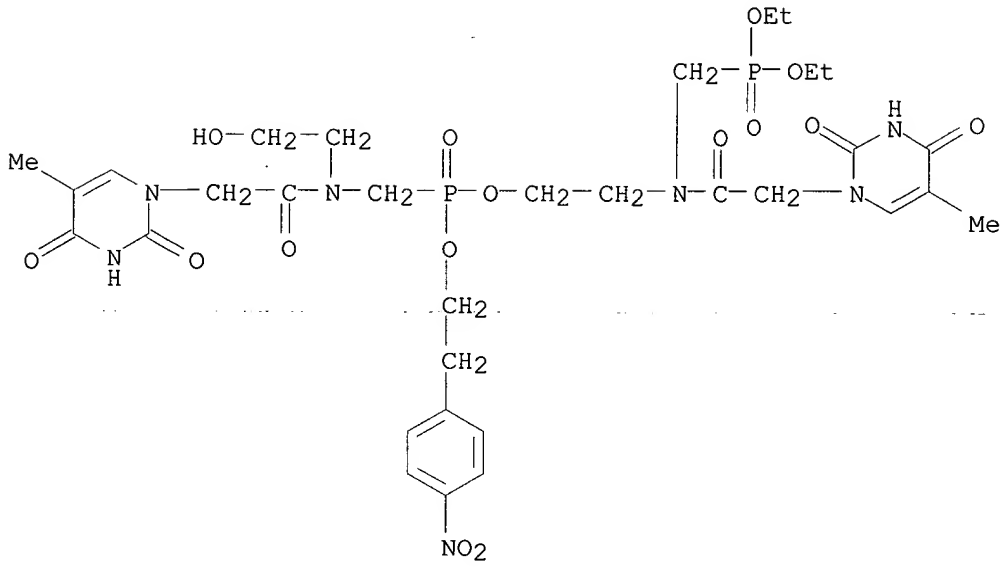
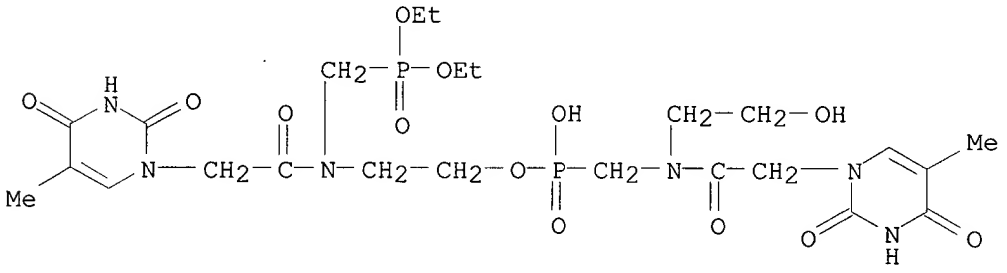


RN 183058-06-2 HCAPLUS
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

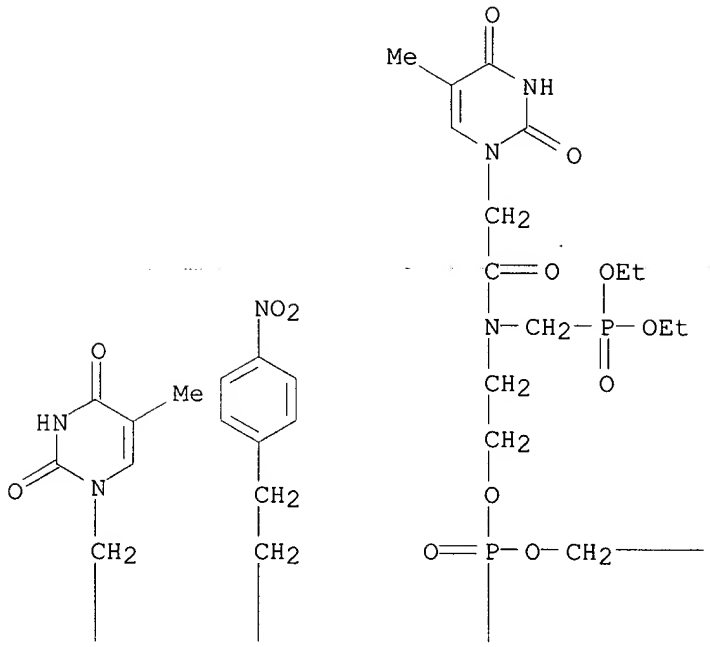


RN 183058-09-5 HCAPLUS
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, mono[2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl] ester (9CI) (CA INDEX NAME)



RN 183058-10-8 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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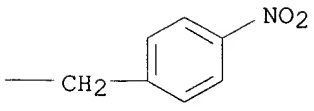

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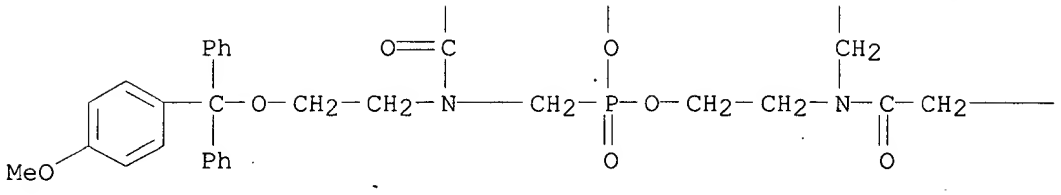

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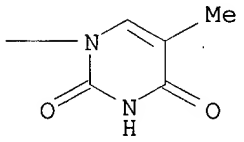

RN 183058-11-9 HCAPLUS
CN Phosphonic acid, [10-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8-(2-hydroxyethyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-9-oxo-5-oxa-2,8-diaza-6-phosphadec-1-yl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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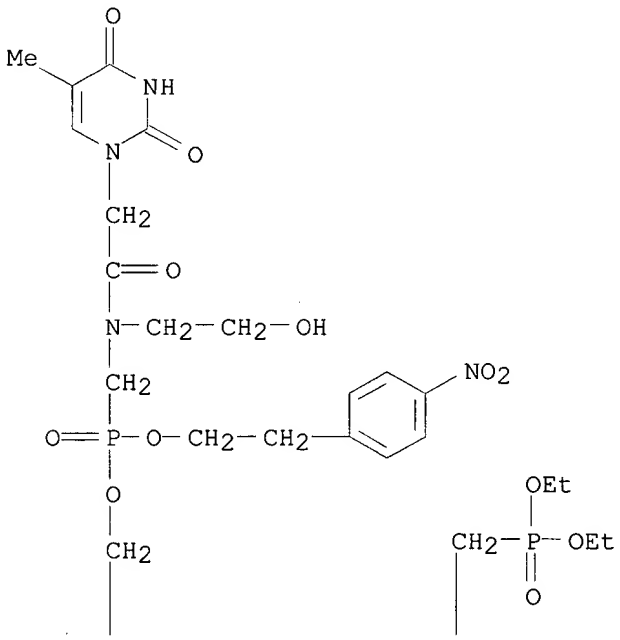

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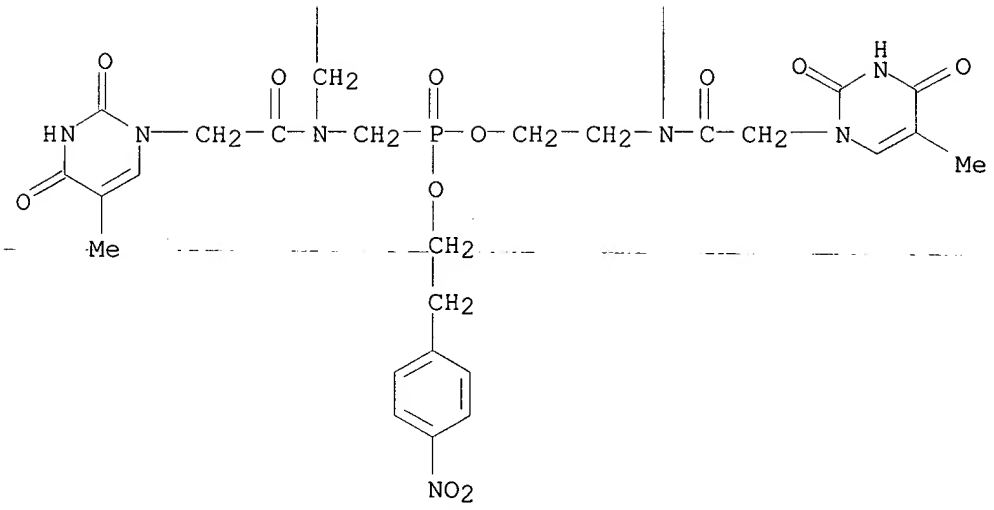

RN 183058-12-0 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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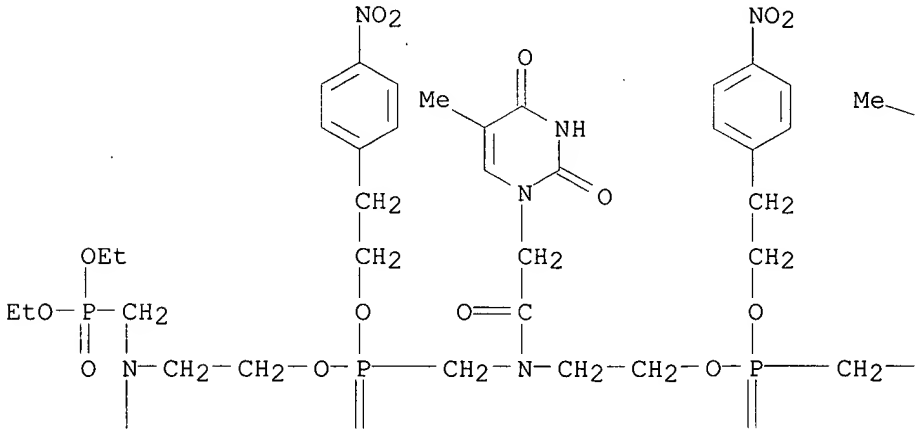

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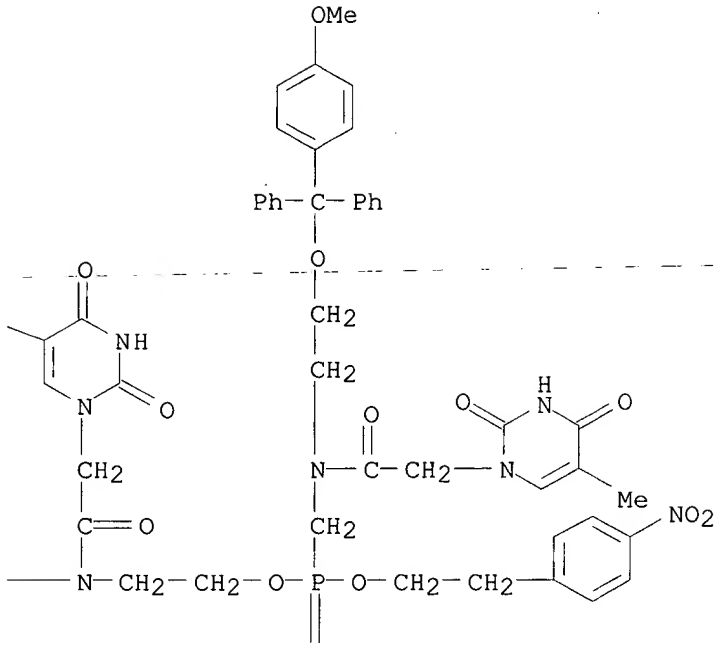

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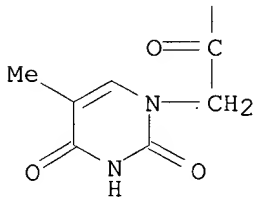

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RN 183058-13-1 HCAPLUS
CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14-(2-hydroxyethyl)-6,12-bis[(4-nitrophenyl)ethoxy]-6,12-dioxido-15-oxo-5,11-dioxa-2,8,14-triaza-6,12-diphosphahexadec-1-yl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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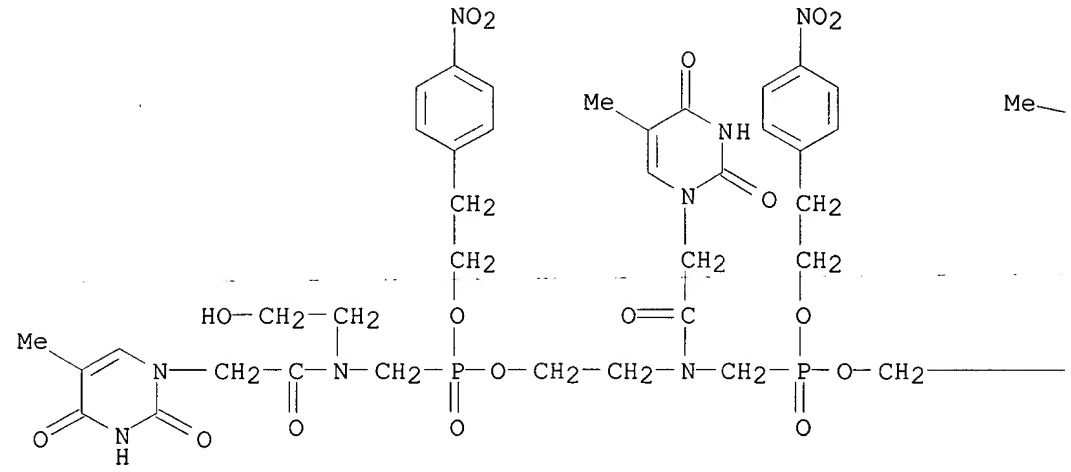

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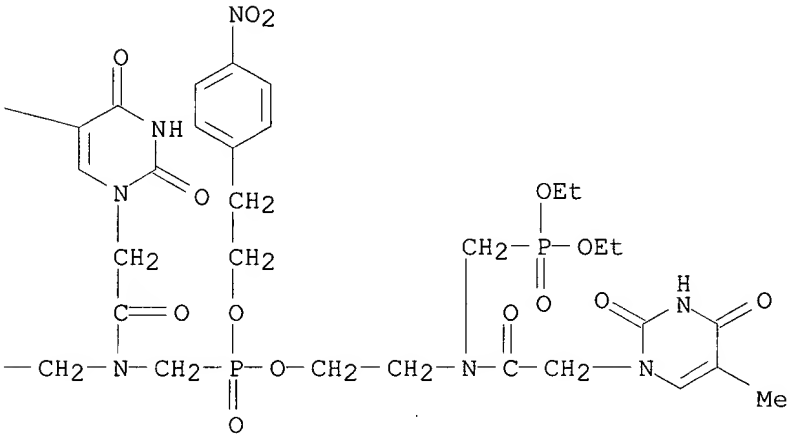

RN 183058-14-2 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

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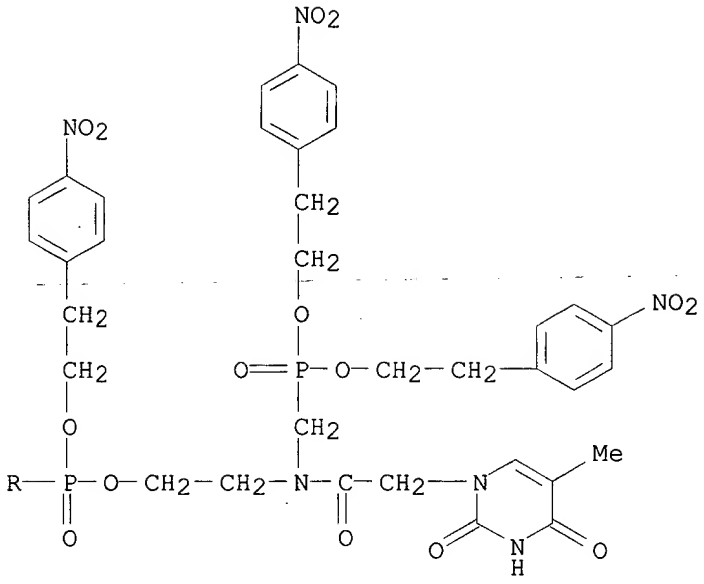

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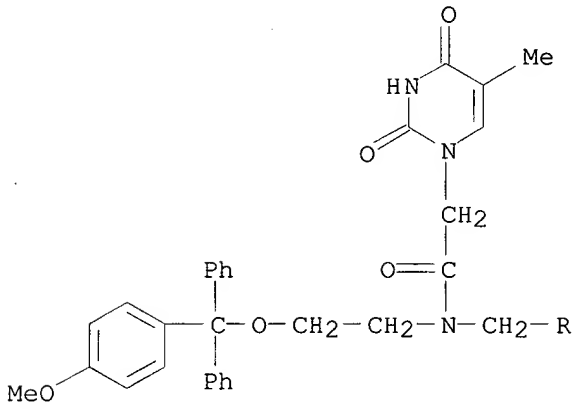

RN 183058-15-3 HCAPLUS
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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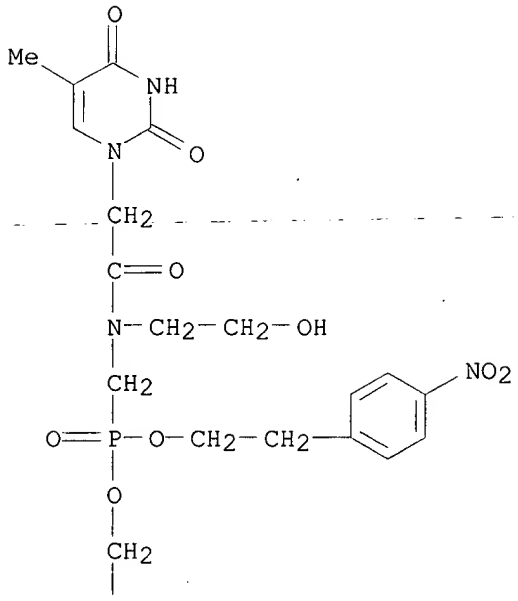

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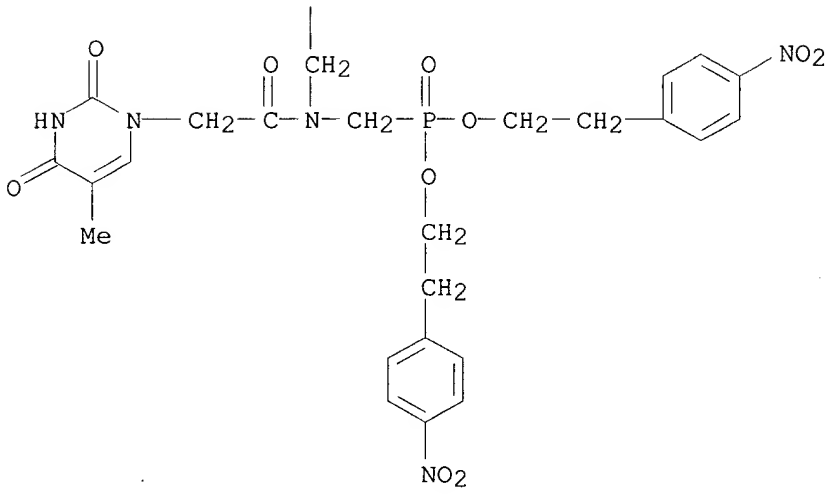

RN 183058-16-4 HCAPLUS
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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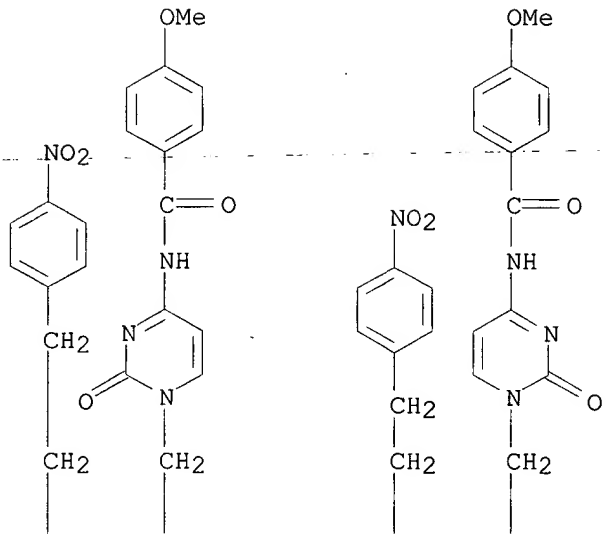

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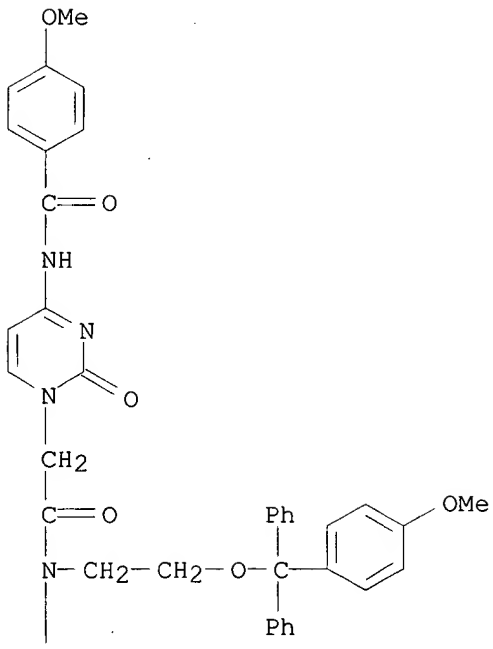

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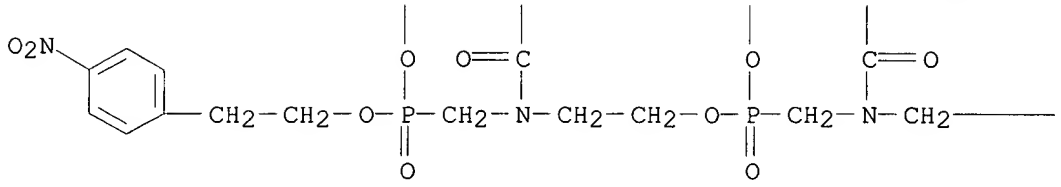

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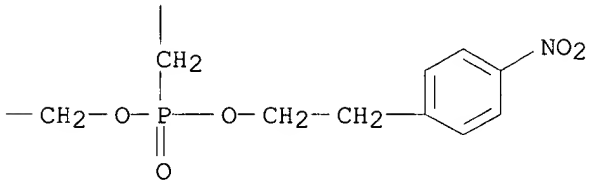

RN 183058-18-6 HCAPLUS
CN Phosphonic acid, [8-(2-hydroxyethyl)-10-[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]-2-[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-9-oxo-5-oxa-2,8-diaza-6-phosphadec-1-yl]-, 2-[[[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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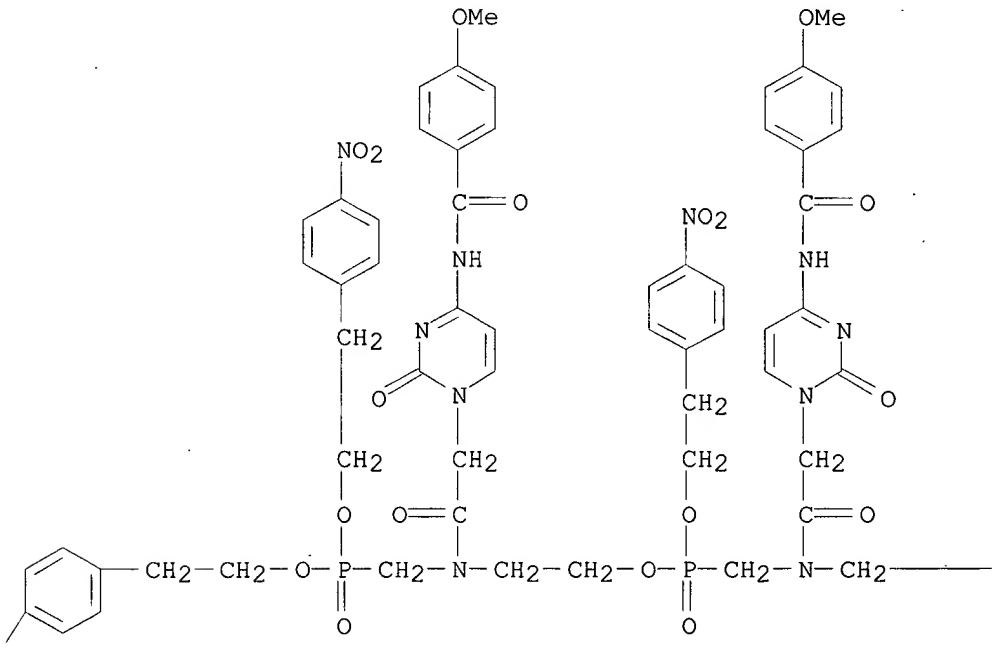

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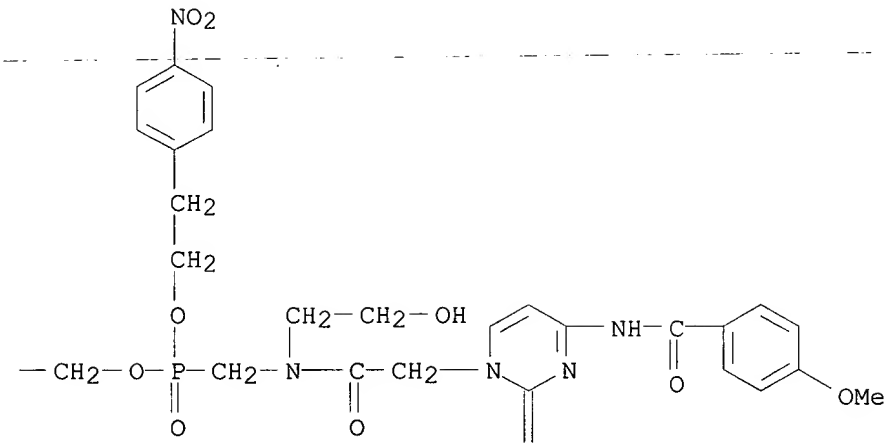

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RN 185670-60-4 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-(4-nitrophenyl)ethyl 2-propenyl ester (9CI) (CA INDEX NAME)

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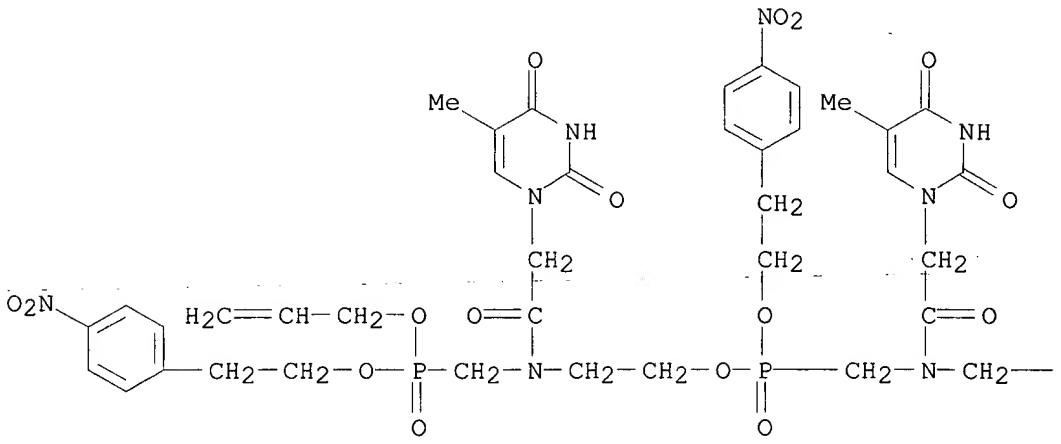

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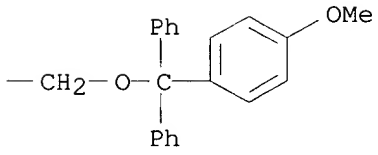

RN 185670-61-5 HCAPLUS

CN Phosphonic acid, [2,8,14-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-18-(4-methoxyphenyl)-6,12-bis[2-(4-nitrophenyl)ethoxy]-6,12-dioxido-18,18-diphenyl-5,11,17-trioxa-2,8,14-triaza-6,12-diphosphaoctadec-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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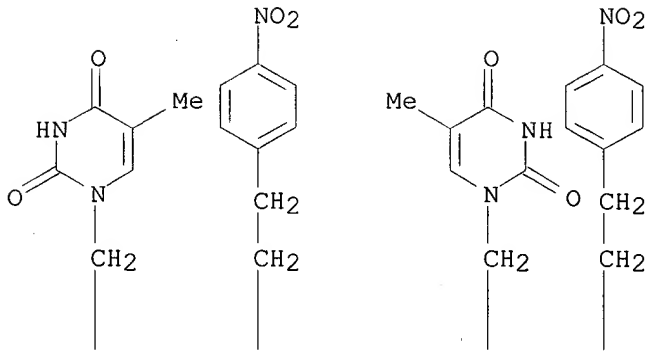

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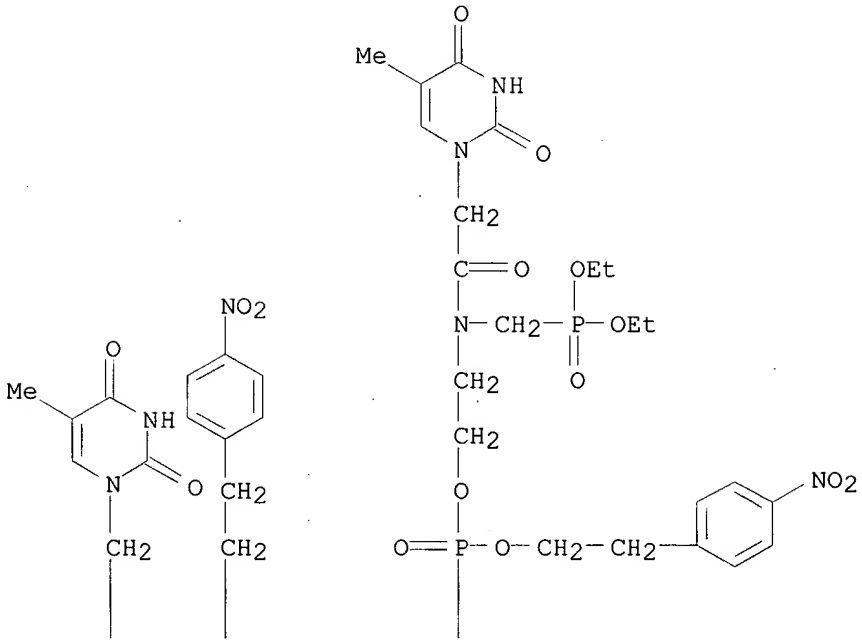

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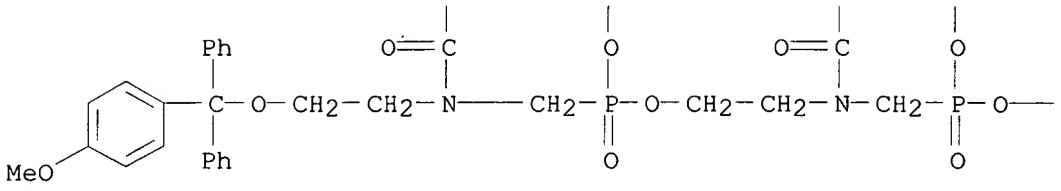

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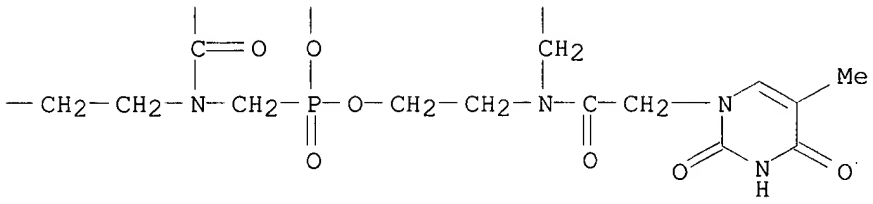

RN 185670-62-6 HCAPLUS

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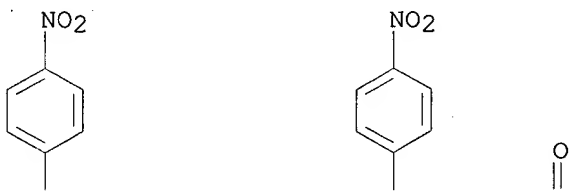

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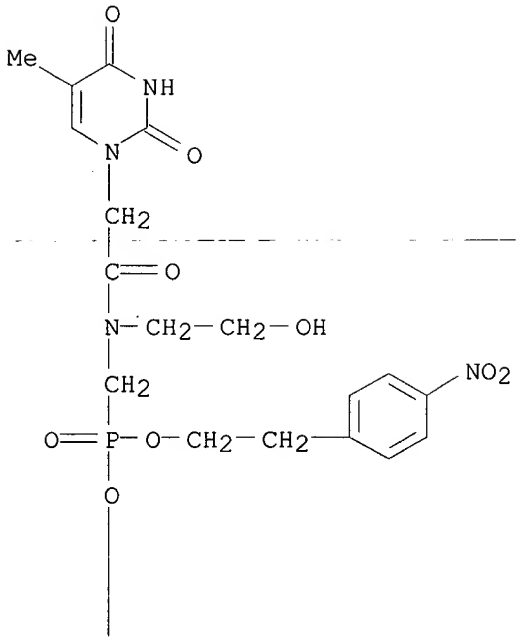

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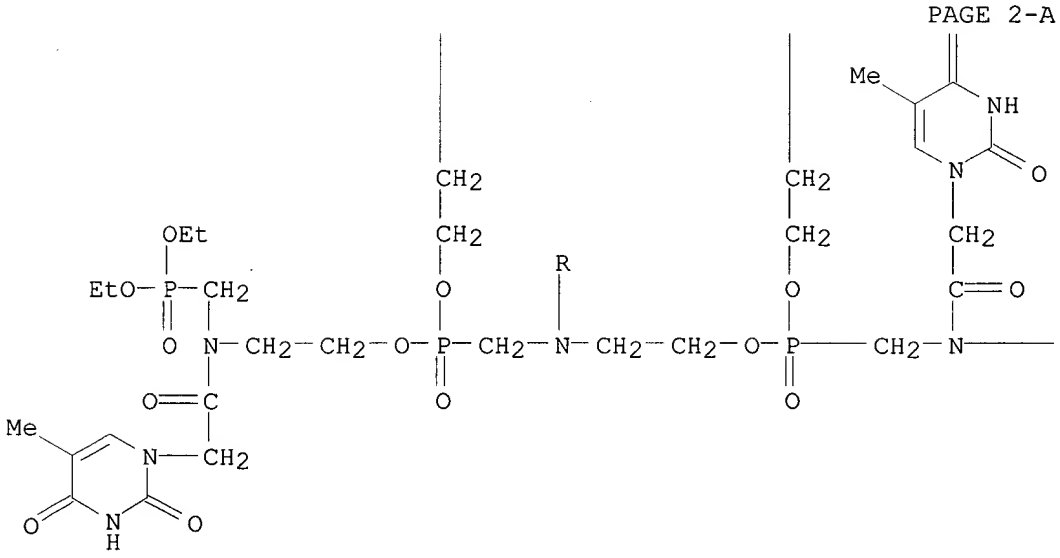

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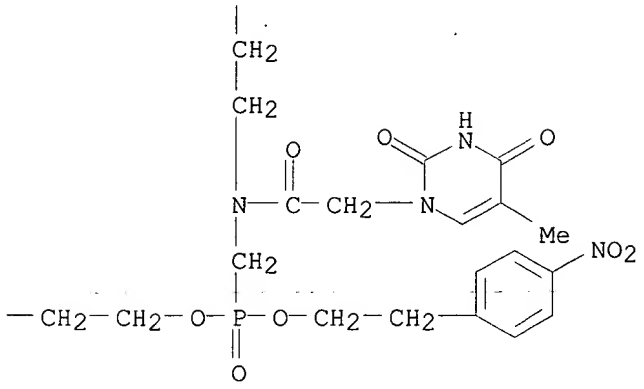

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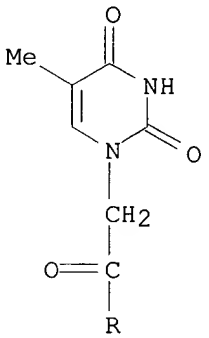

RN 185670-63-7 HCAPLUS
CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12-dihydroxy-14-(2-hydroxyethyl)-6,12-dioxido-15-oxo-5,11-dioxa-2,8,14-triaza-6,12-diphosphahexadec-1-yl]-, mono[3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-hydroxy-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl] ester (9CI) (CA INDEX NAME)

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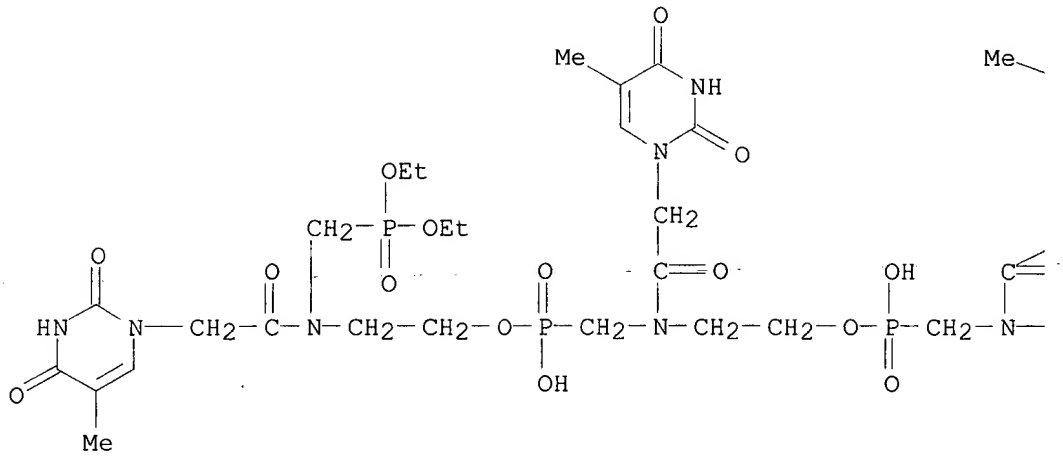

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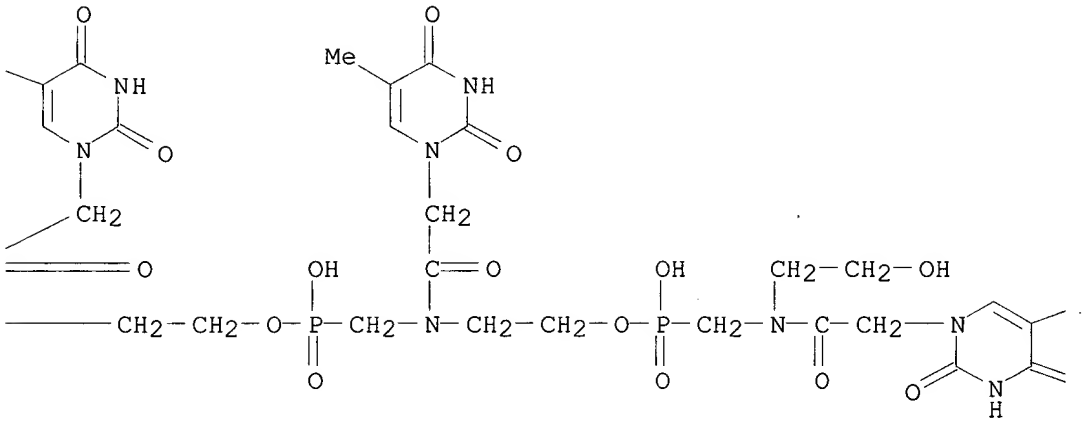

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RN 185670-64-8 HCAPLUS
CN Phosphonic acid, [2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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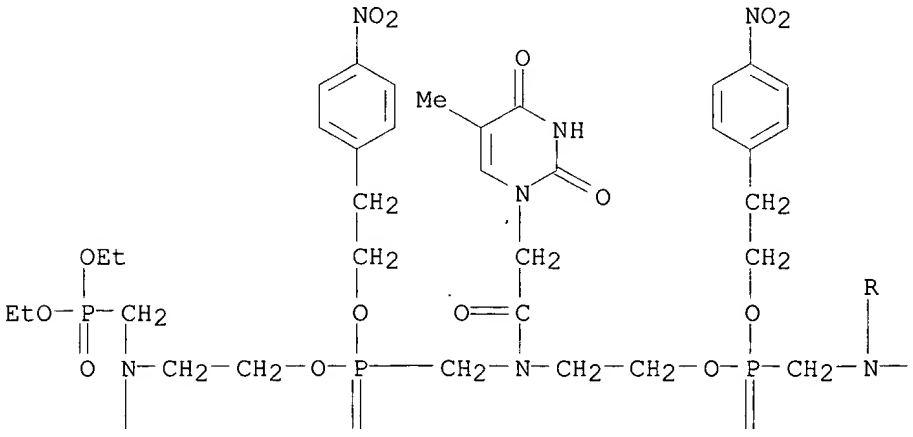

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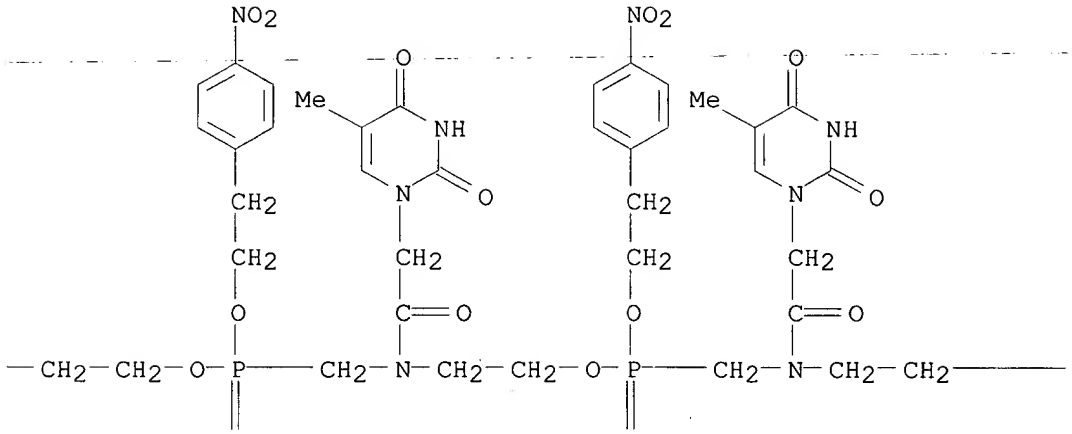

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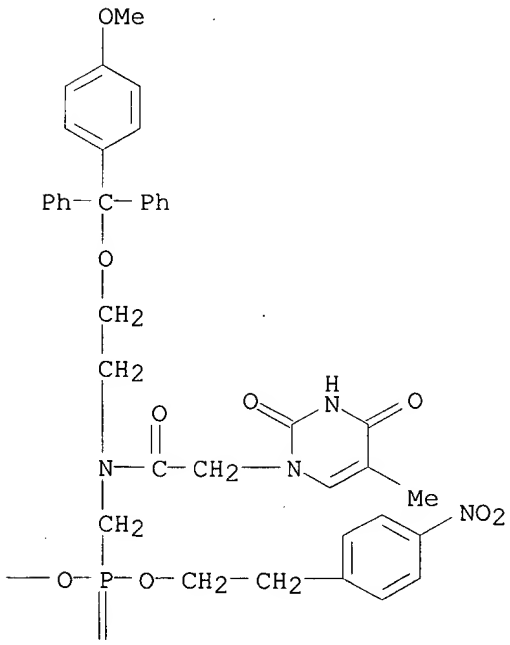

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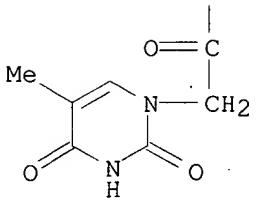

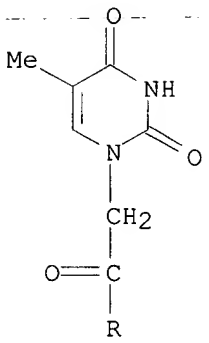

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RN 185670-65-9 HCAPLUS
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl][2-[(4-methoxyphenyl)diphenylmethoxy]ethyl]amino]methyl]-, 2-[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl][[hydroxy[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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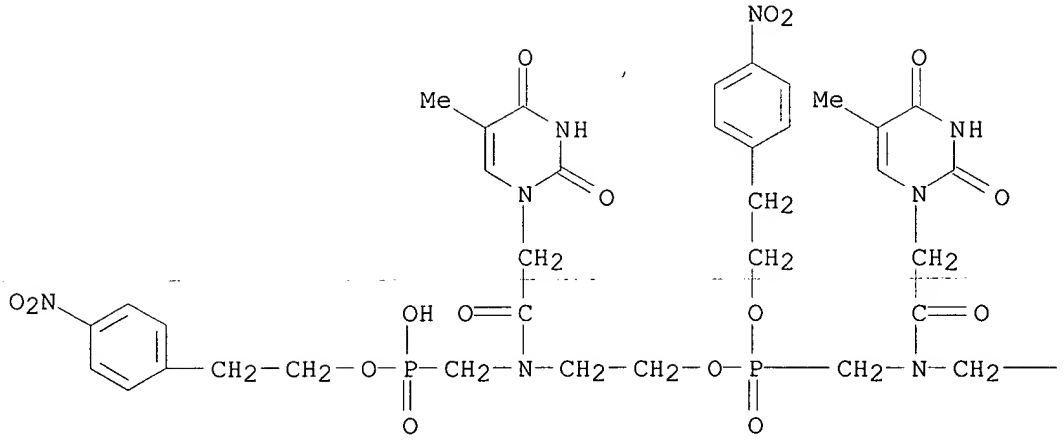

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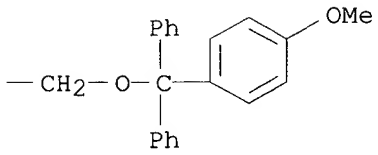

RN 185670-66-0 HCAPLUS

CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14-(2-hydroxyethyl)-6,12-bis[2-(4-nitrophenyl)ethoxy]-6,12-dioxido-15-oxo-5,11-dioxa-2,8,14-triaza-6,12-diphosphahexadec-1-yl]-, 3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-17-ethoxy-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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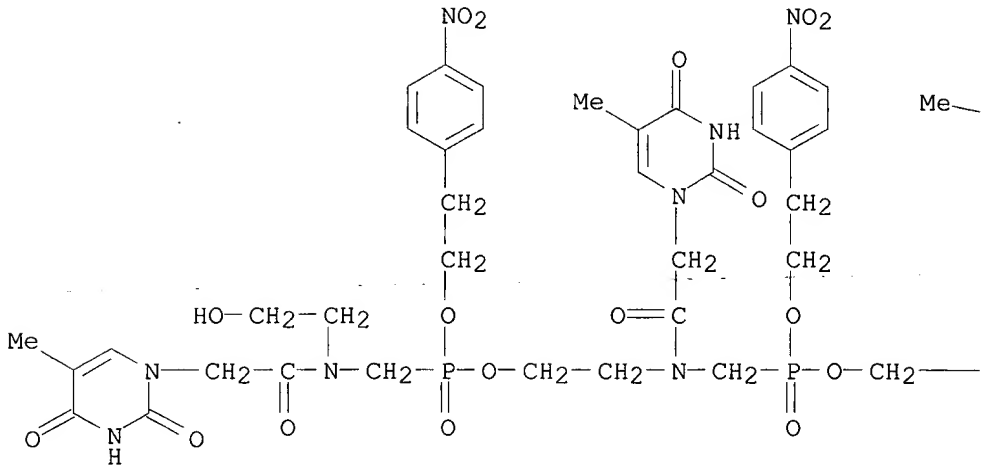

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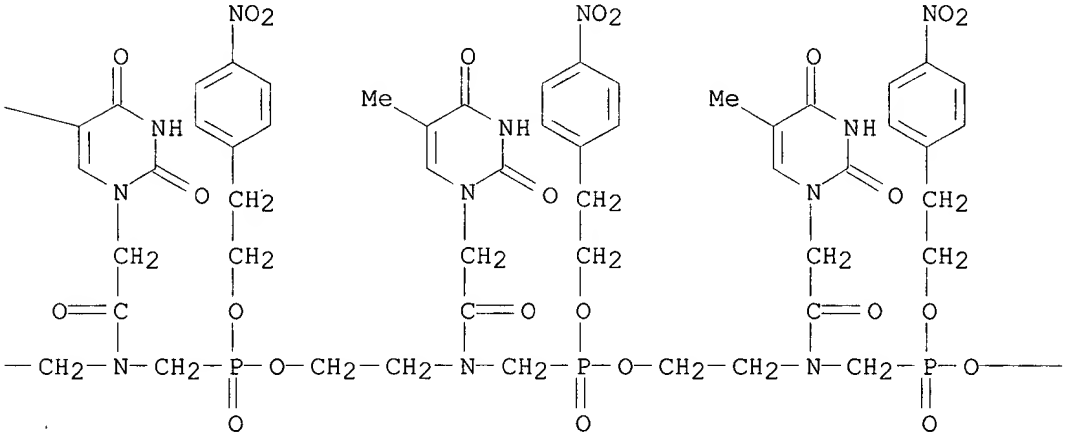

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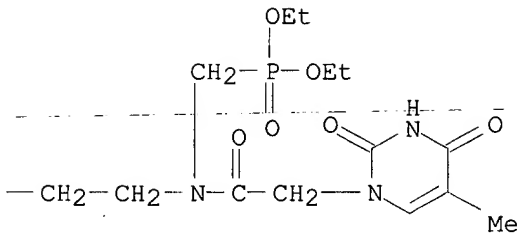

RN 185670-67-1 HCAPLUS
CN Phosphonic acid, [10-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8-(2-hydroxyethyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-5-oxa-2,8-diaza-6-phosphadec-1-yl]-, 2-(4-nitrophenyl)ethyl 2-propenyl ester (9CI) (CA INDEX NAME)

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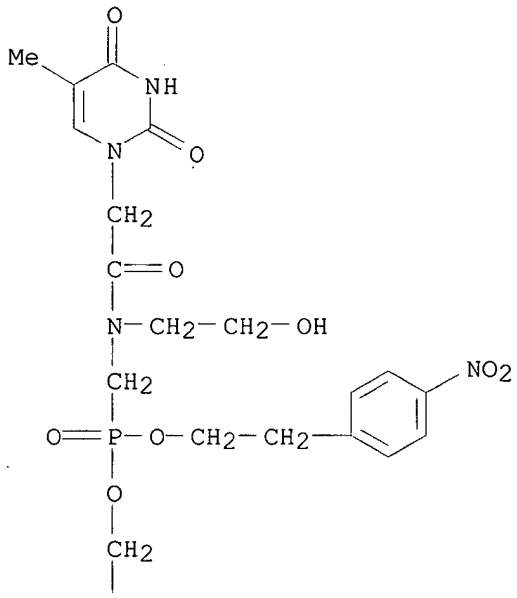

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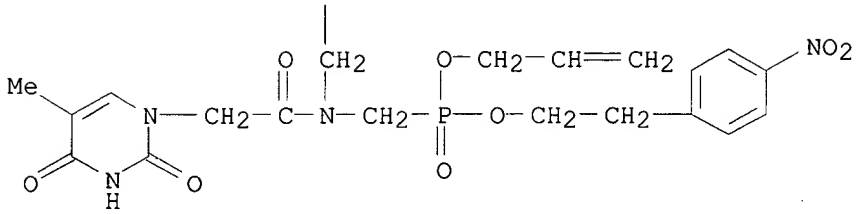

RN 185670-68-2 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl][[hydroxy[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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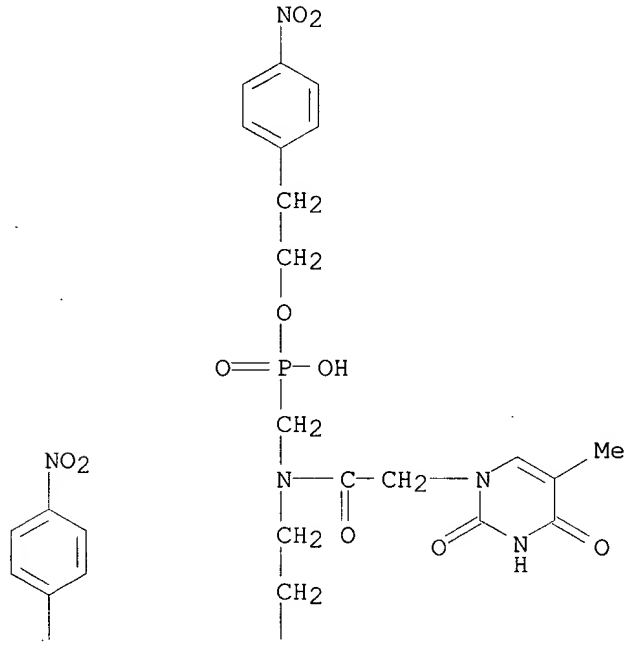

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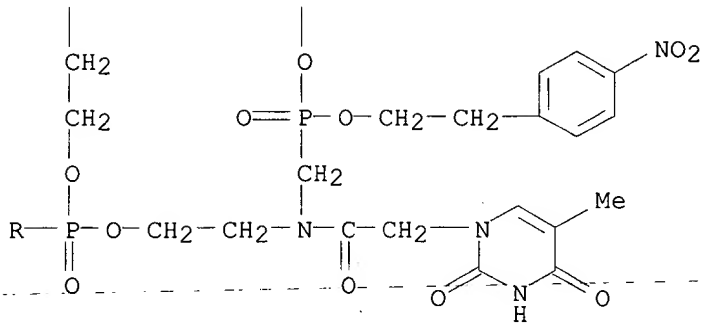

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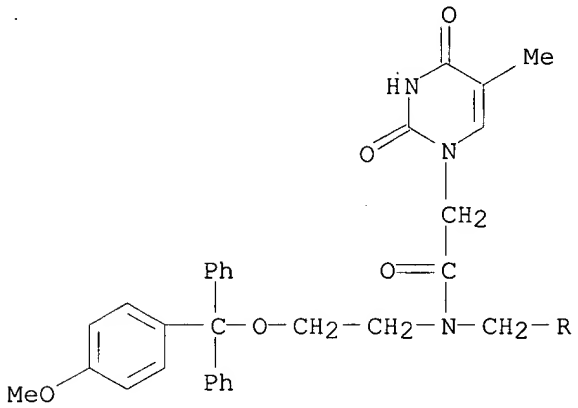

RN 185670-69-3 HCAPLUS
CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12-dihydroxy-14-(2-hydroxyethyl)-6,12-dioxido-15-oxo-5,11-dioxa-2,8,14-triaza-6,12-diphosphahexadec-1-yl]-, mono[3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-17-ethoxy-5,11-dihydroxy-5,11-dioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl] ester (9CI) (CA INDEX NAME)

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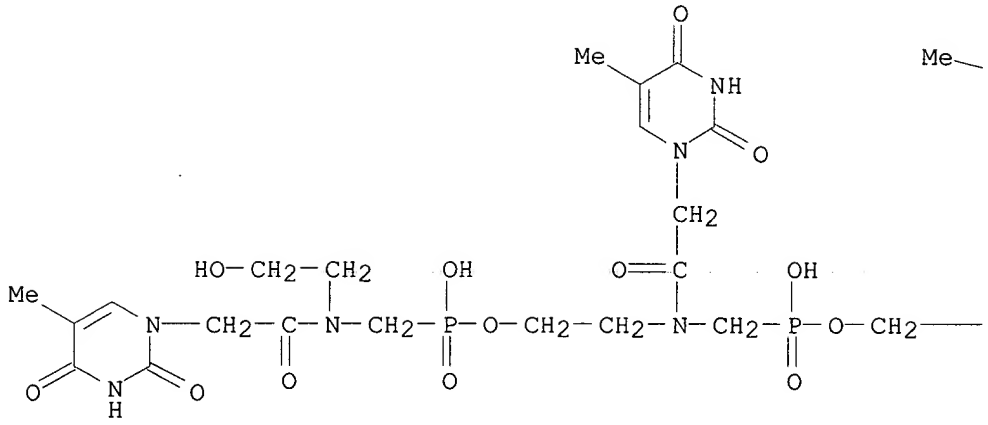

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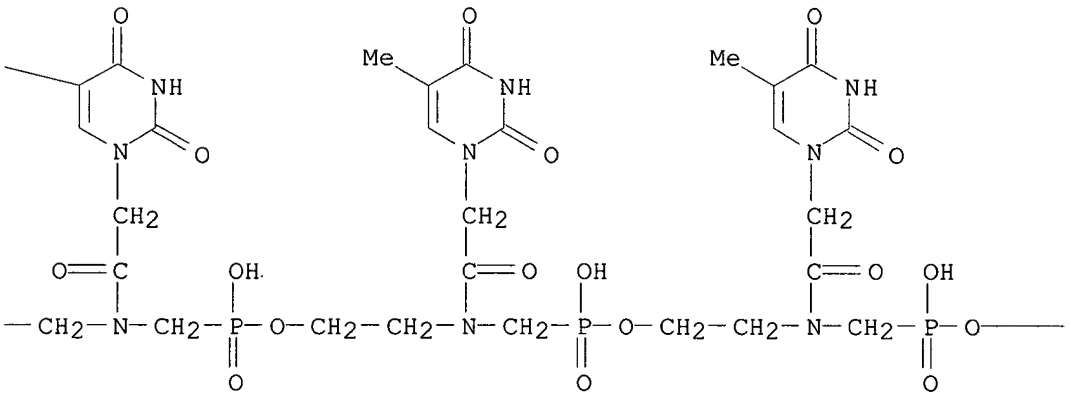

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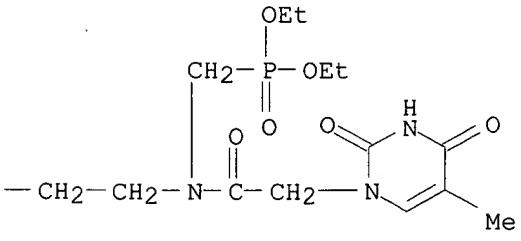

RN 185670-70-6 HCAPLUS
CN Phosphonic acid, [2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, 2-(4-nitrophenyl)ethyl 3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-17-ethoxy-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl ester (9CI) (CA INDEX NAME)

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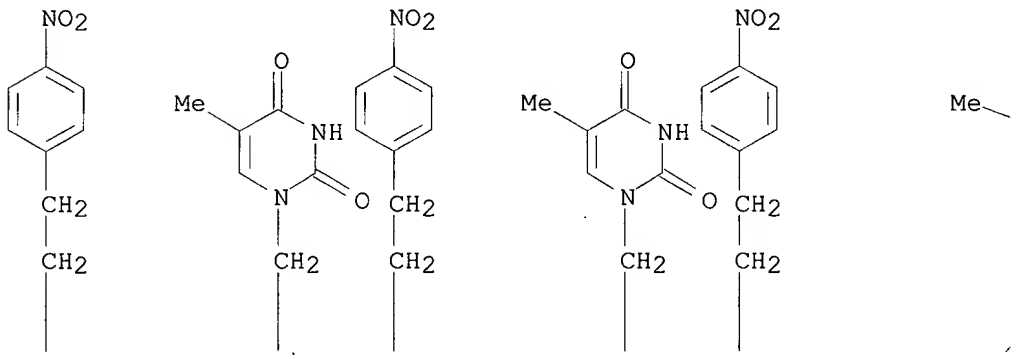

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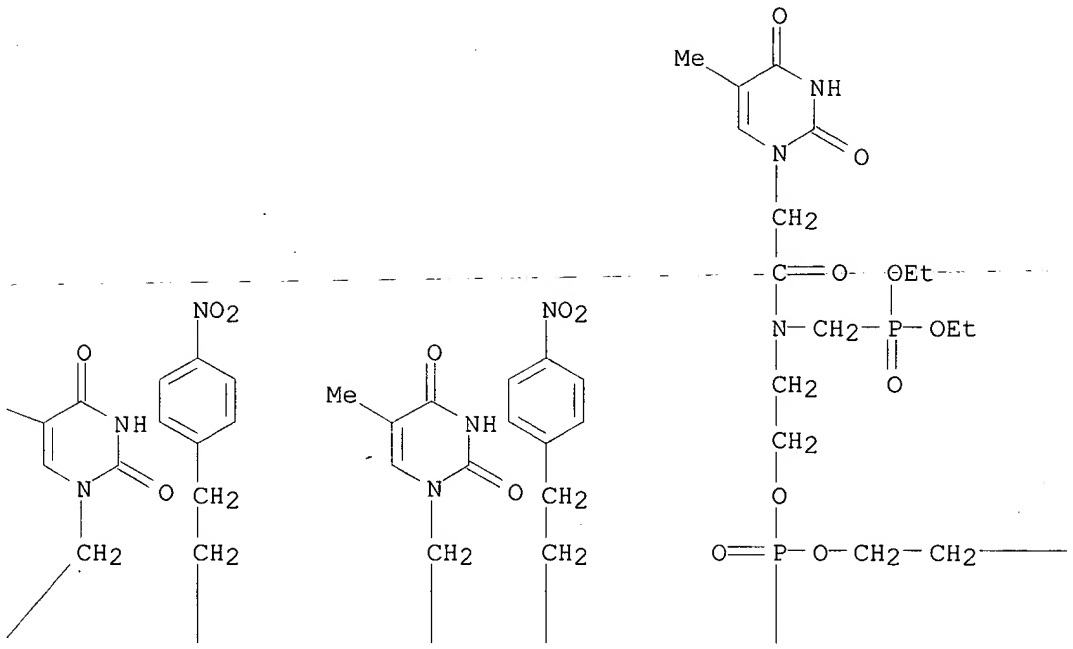

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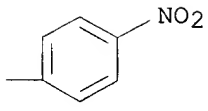

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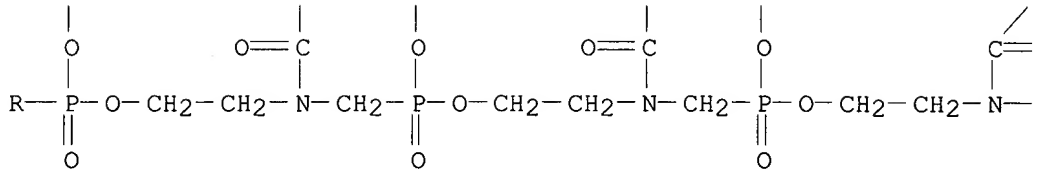

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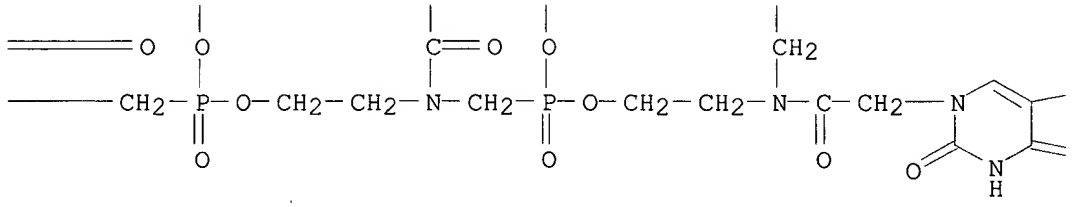

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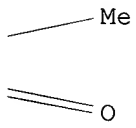

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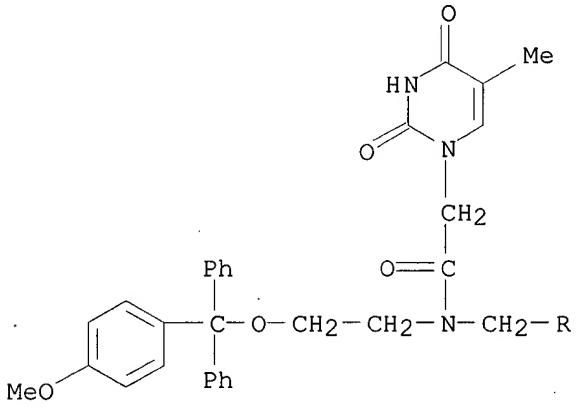

RN 185670-71-7 HCAPLUS
CN Phosphonic acid, [22-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8,14-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-20-(2-hydroxyethyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-3,12,18-trioxido-21-oxo-5,11,17-trioxa-2,8,14,20-tetraaza-6,12,18-triphosphadocos-1-yl]-, 2-(4-nitrophenyl)ethyl 3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-

pyrimidinyl)acetyl]-17-ethoxy-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl ester (9CI) (CA INDEX NAME).

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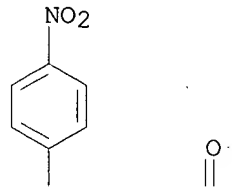

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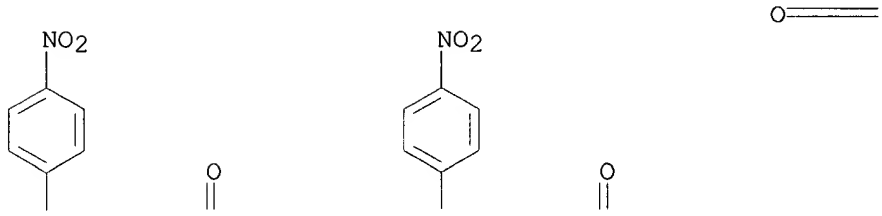

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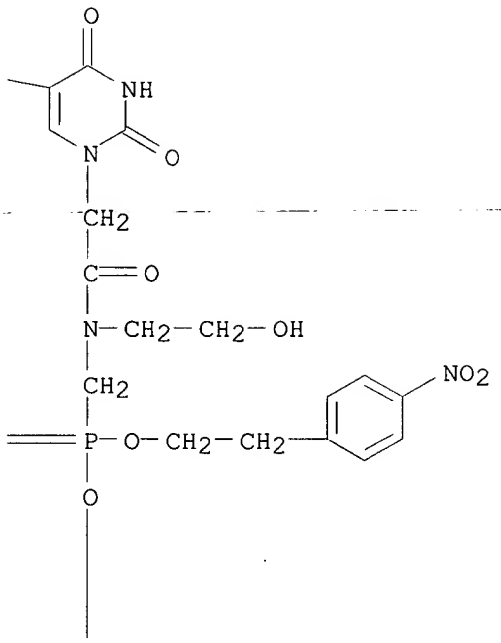

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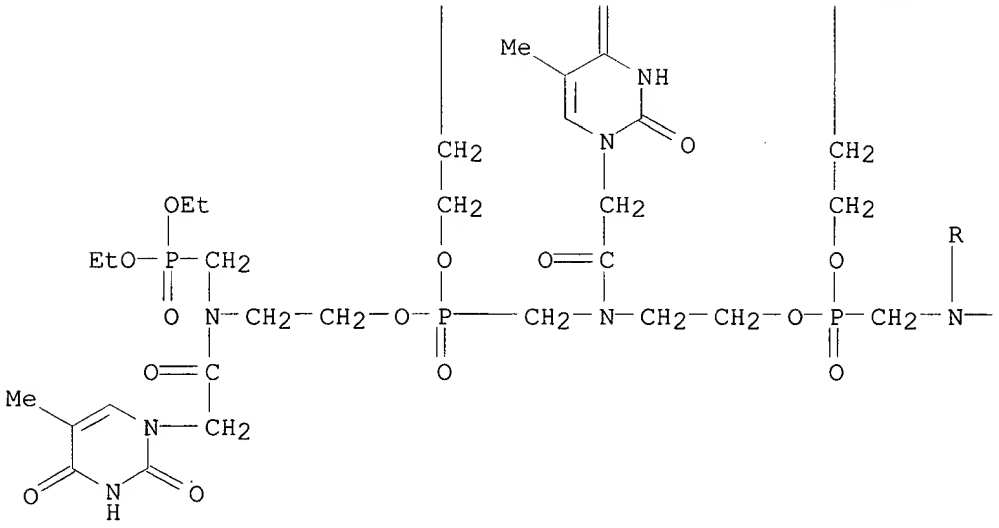

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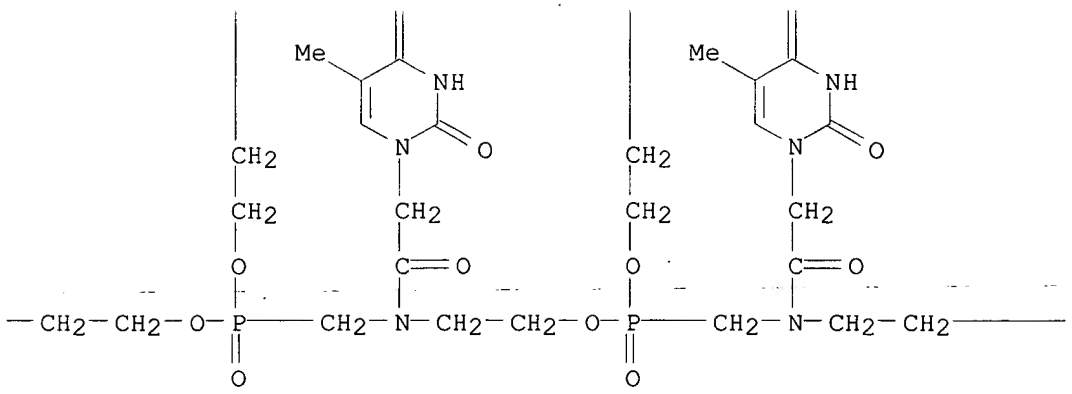

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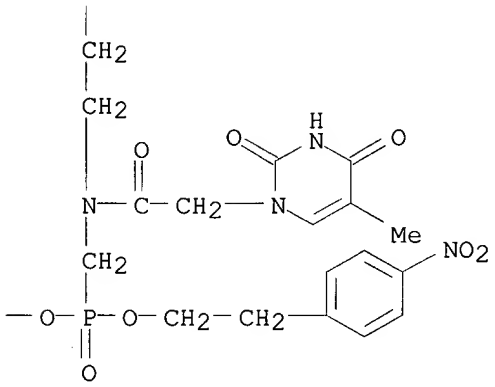

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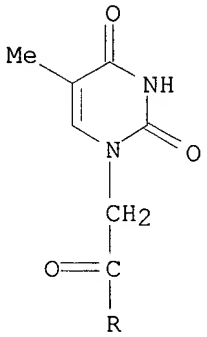

RN 185670-72-8 HCAPLUS
CN Phosphonic acid, [22-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8,14-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12,18-trihydroxy-20-(2-hydroxyethyl)-6,12,18-trioxido-21-oxo-5,11,17-trioxa-2,8,14,20-tetraaza-6,12,18-triphosphadocos-1-yl]-,

mono[3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-17-ethoxy-5,11-dihydroxy-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl] ester (9CI) (CA INDEX NAME)

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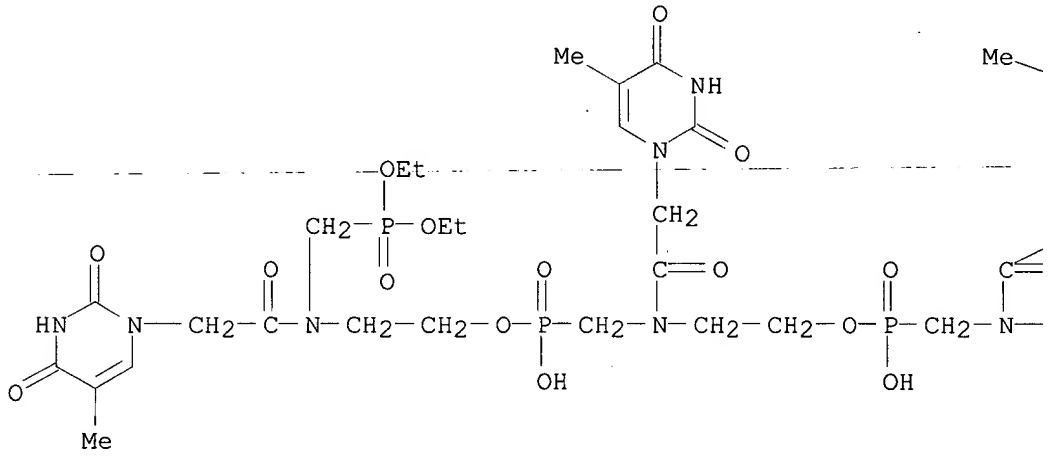

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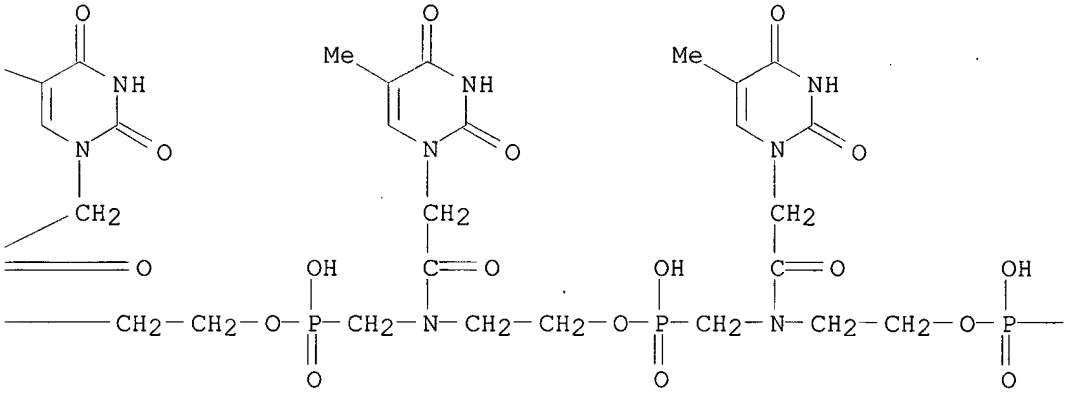

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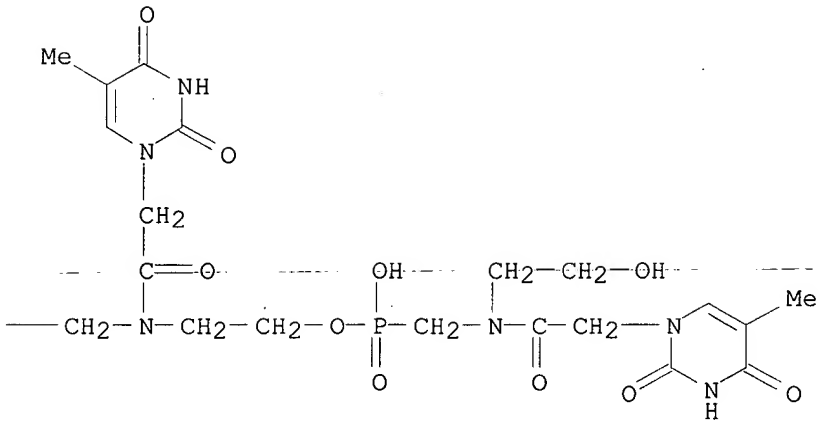

RN 185670-95-5 HCAPLUS
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-(4-nitrophenyl)ethyl 2-propenyl ester (9CI) (CA INDEX NAME)

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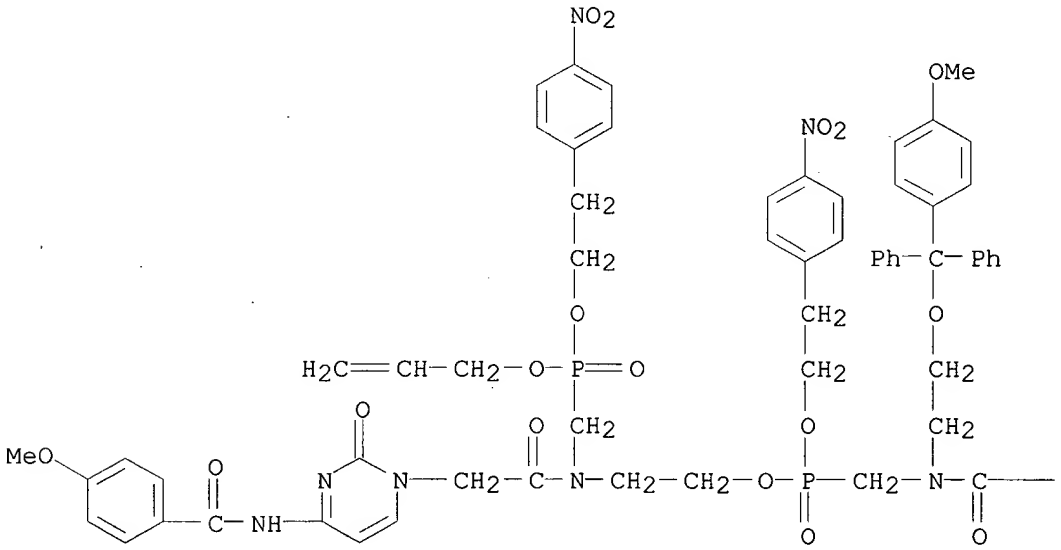

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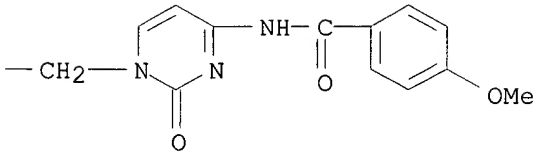

RN 185670-96-6 HCAPLUS
CN Phosphonic acid, [[(2-hydroxyethyl)[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]methyl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[[2-(4-nitrophenyl)ethoxy](2-propenyloxy)phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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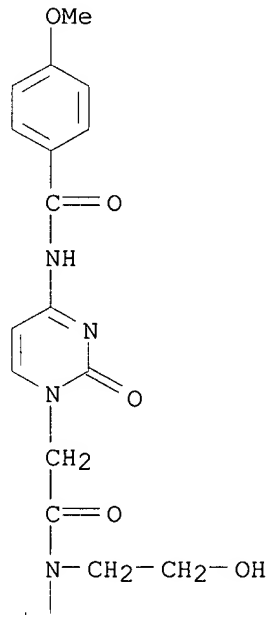

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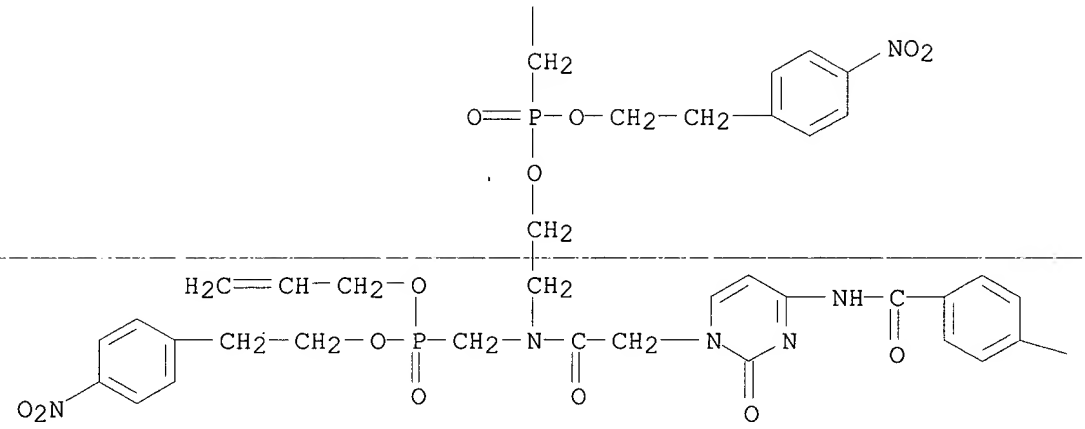

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RN 185670-97-7 HCAPLUS

CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[[2-(4-nitrophenyl)ethoxy](2-propenyloxy)phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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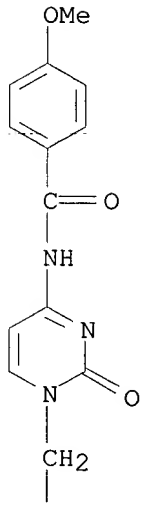

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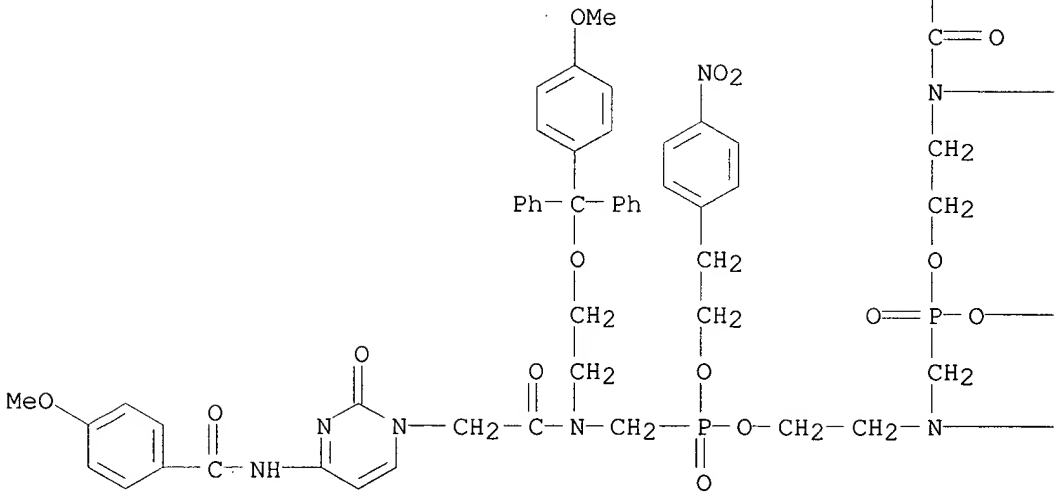

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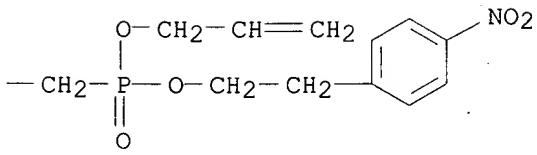

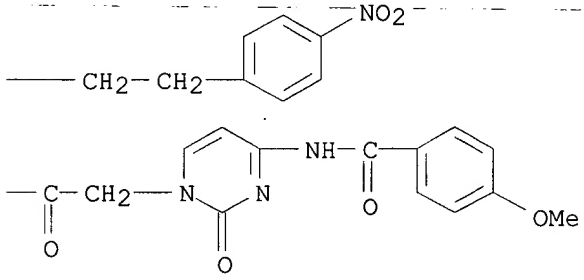

RN 185670-98-8 HCAPLUS
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[hydroxy[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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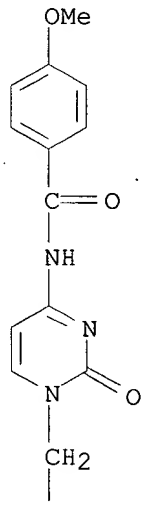

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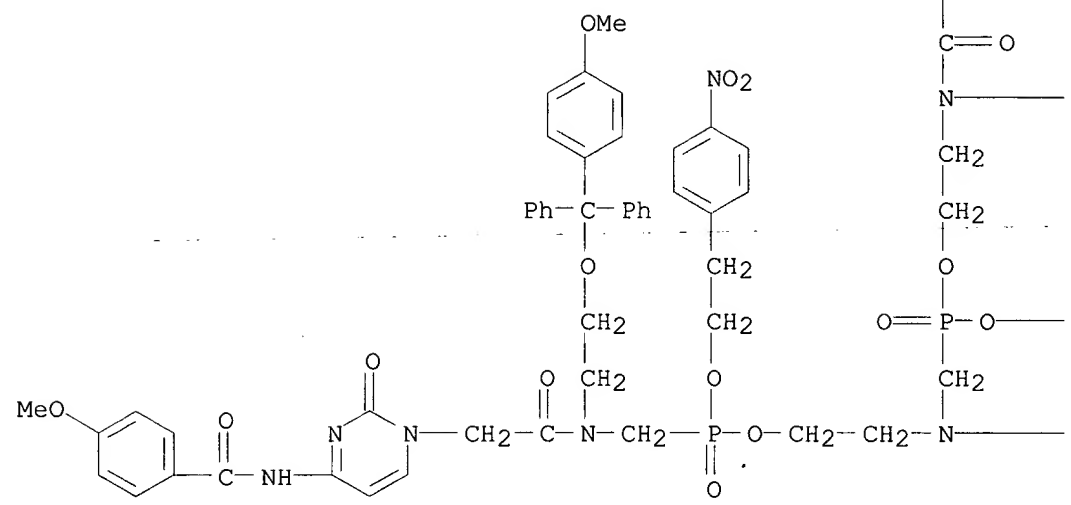

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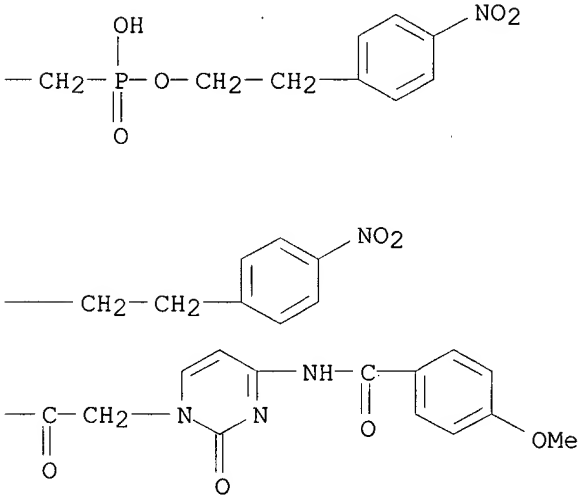
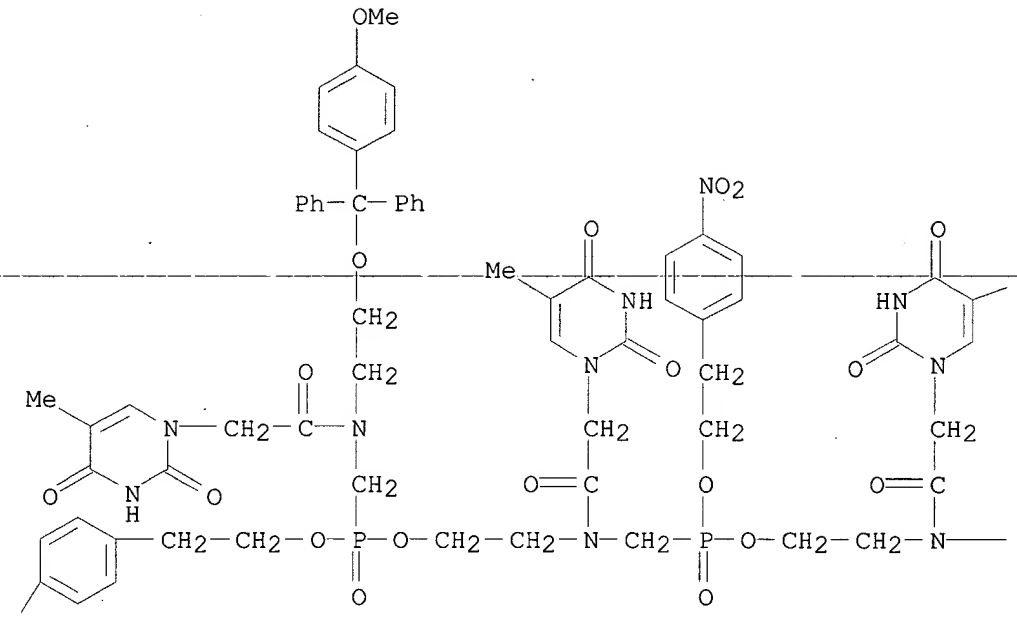


RN 185670-99-9 HCAPLUS

CN Phosphonic acid, [8,14,20-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-2-[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, 11-ethoxy-3,9-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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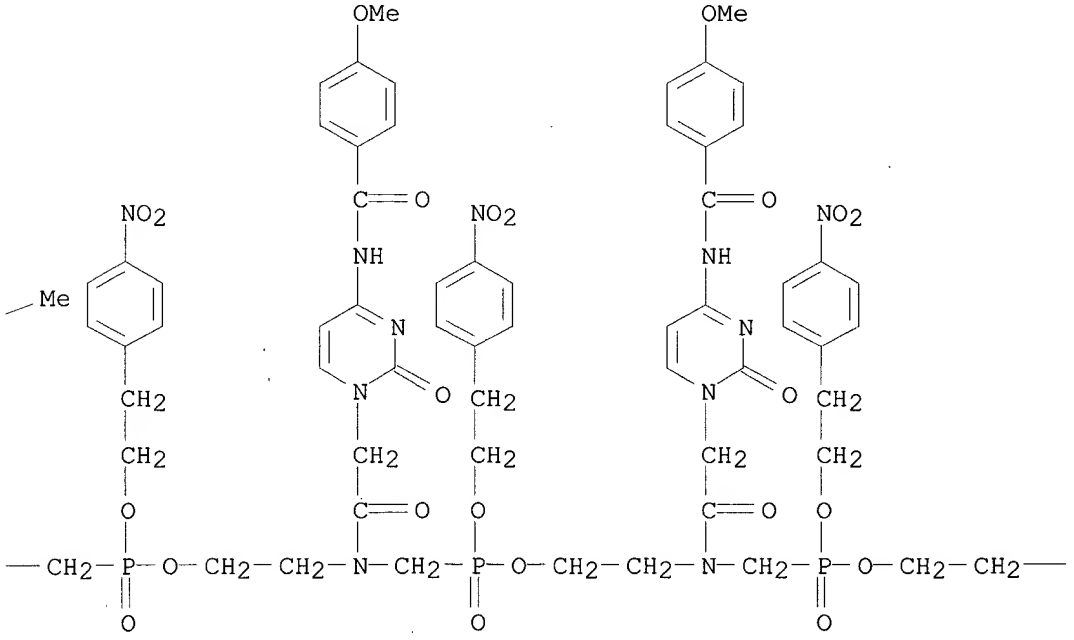

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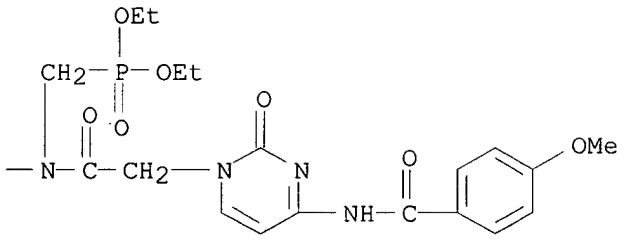
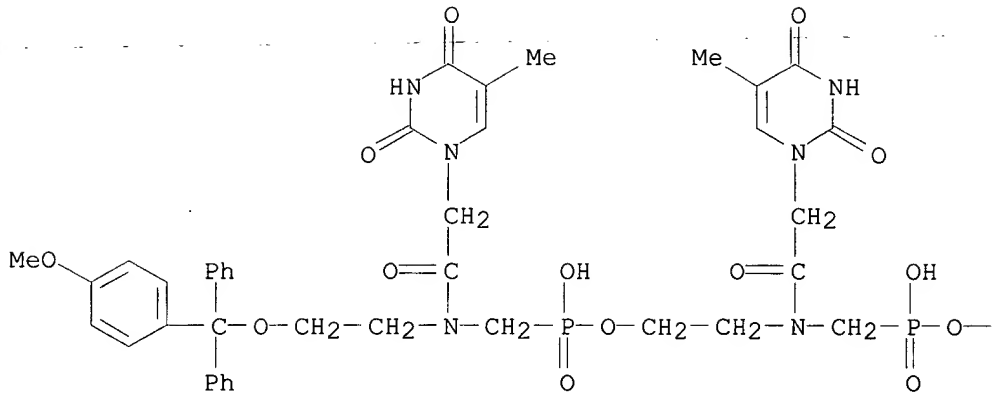


PAGE 2-A

RN 185671-00-5 HCAPLUS
CN Phosphonic acid, [2,8,14-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12-dihydroxy-18-(4-methoxyphenyl)-6,12-dioxido-18,18-diphenyl-5,11,17-trioxa-2,8,14-triaza-6,12-diphosphaoctadec-1-yl]-, mono[5,11,17,17-tetrahydroxy-3,9,15-tris[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-5,11,17-trioxido-6,12-dioxa-3,9,15-triaza-5,11,17-triphosphaheptadec-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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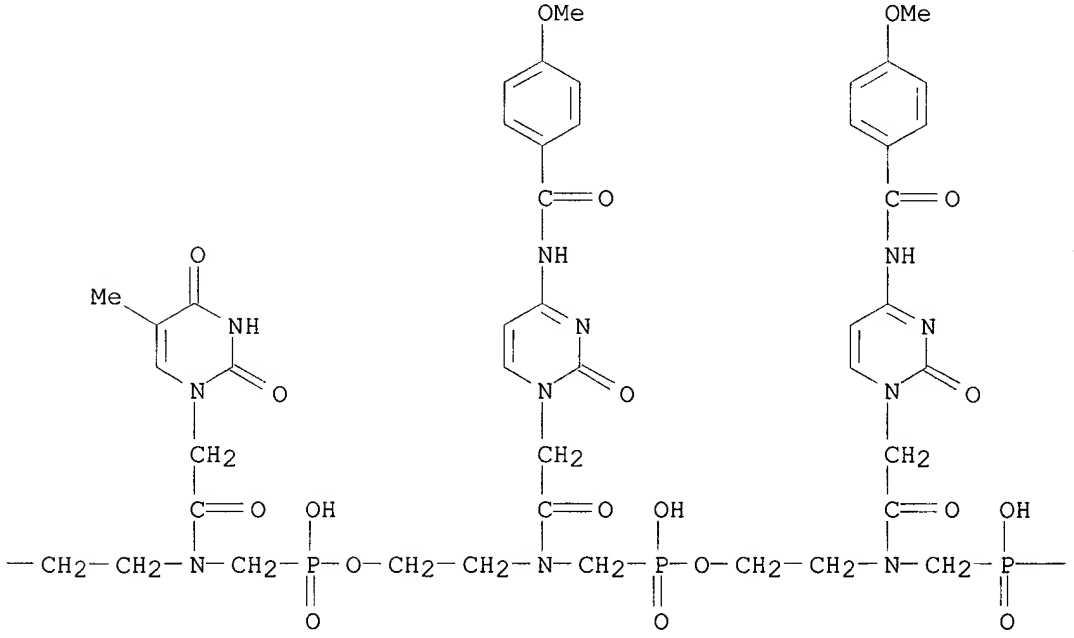

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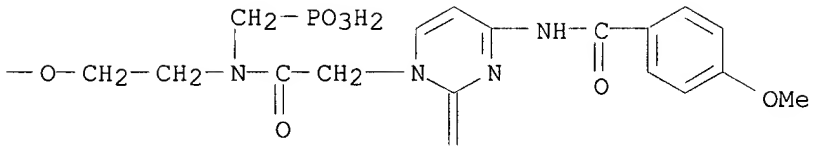
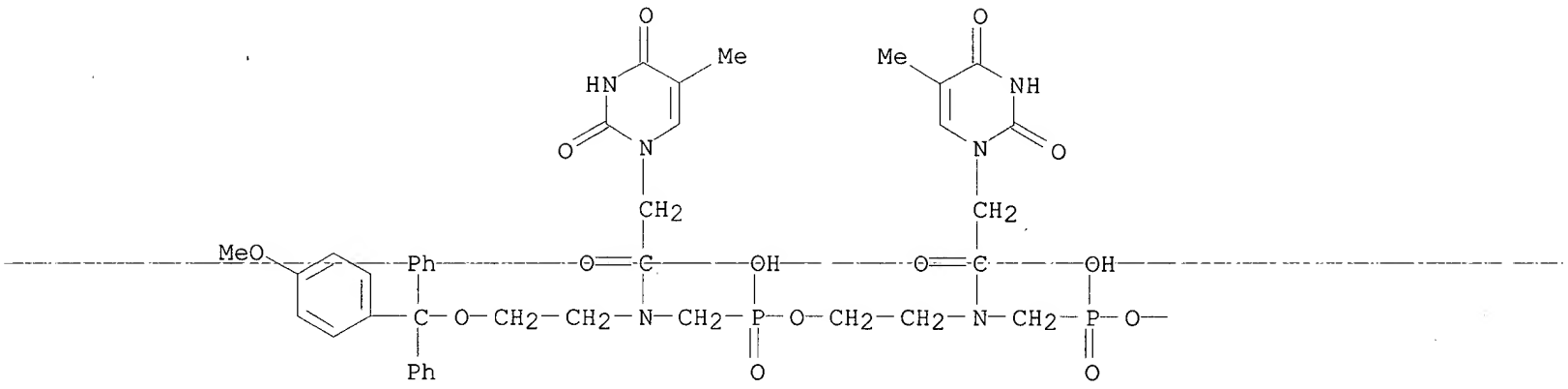


PAGE 2-C

RN 185671-01-6 HCAPLUS
CN Phosphonic acid, [2-[(4-amino-2-oxo-1(2H)-pyrimidinyl)acetyl]-8,14,20-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12,18-trihydroxy-24-(4-methoxyphenyl)-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, mono[3,9-bis[(4-amino-2-oxo-1(2H)-pyrimidinyl)acetyl]-5,11,11-trihydroxy-5,11-dioxido-6-oxa-3,9-diaza-5,11-diphosphaundec-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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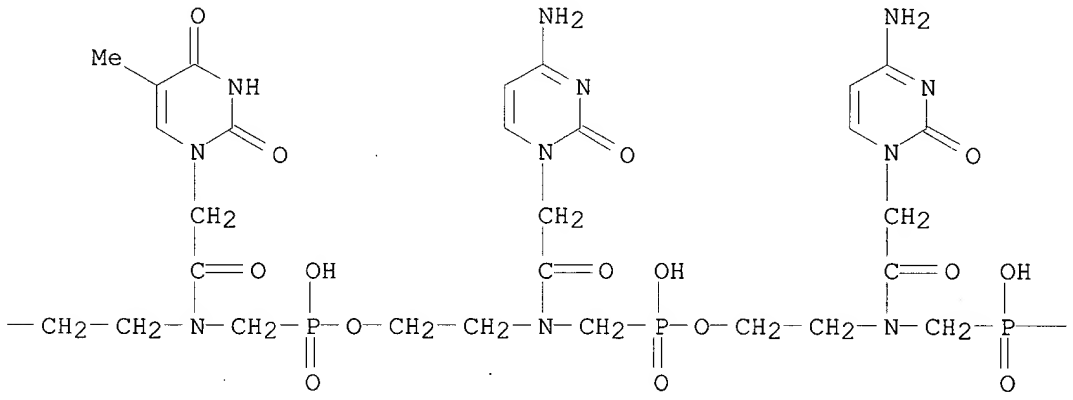

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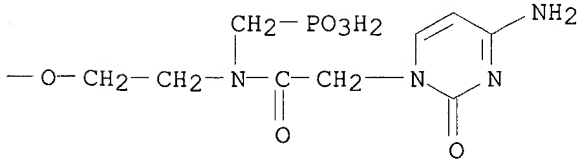

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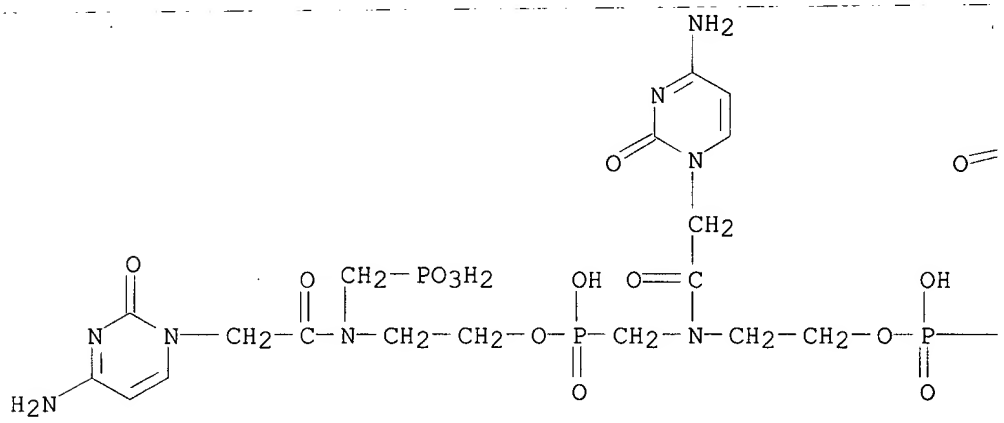
PAGE 1-A



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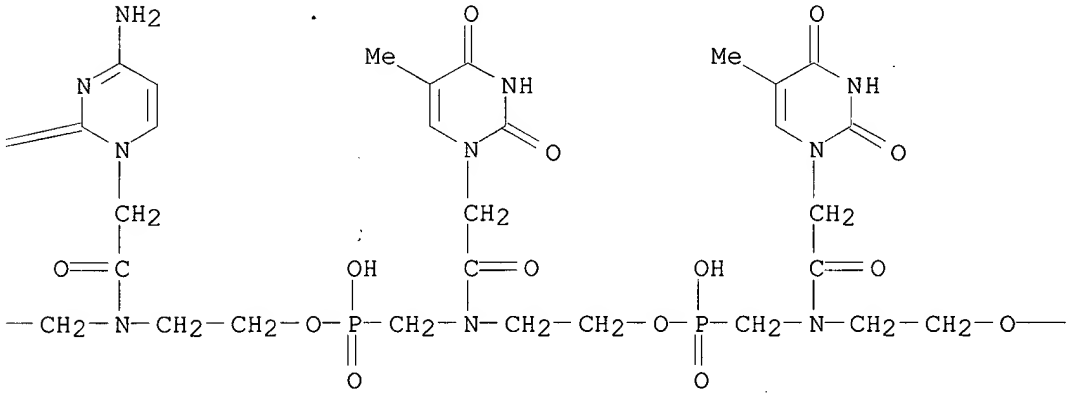

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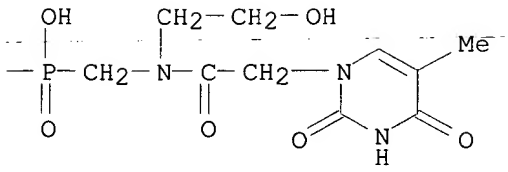
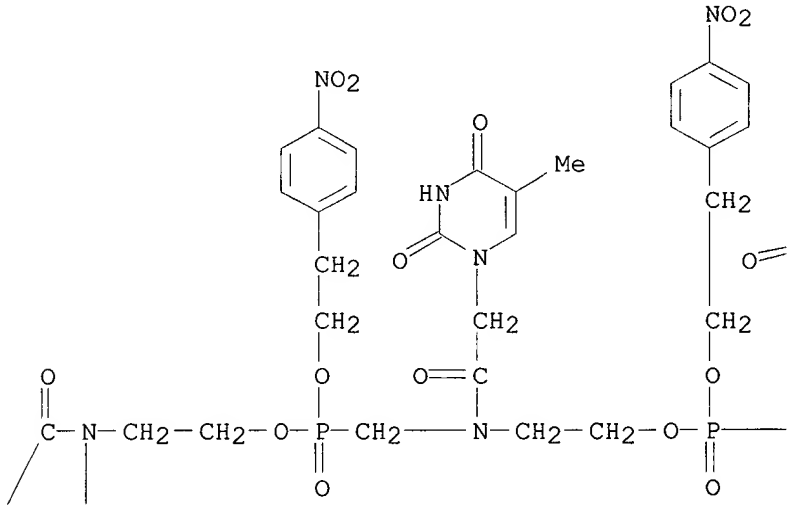


RN 185671-03-8 HCAPLUS
CN Phosphonic acid, [2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8,14,20-tris[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14-(4-nitrophenyl)-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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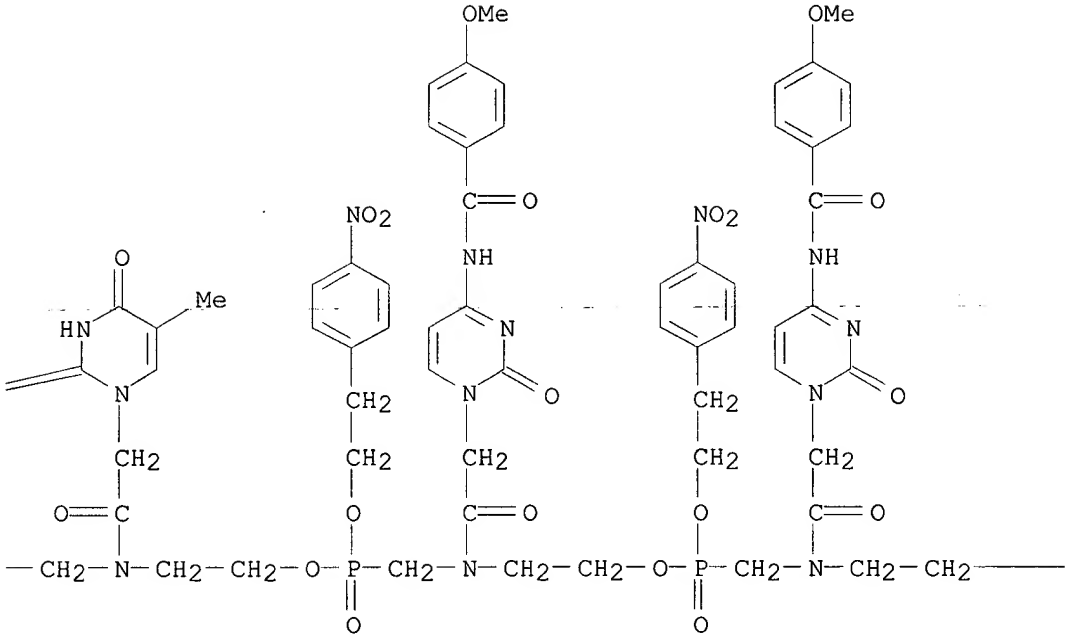

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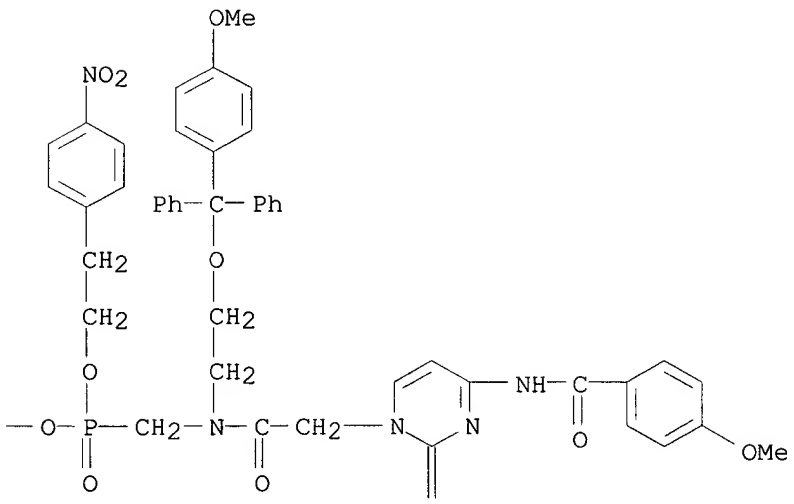

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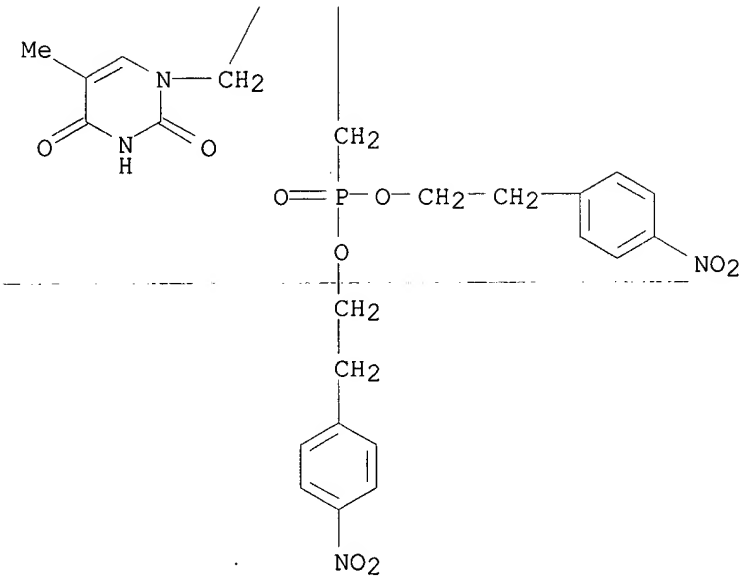

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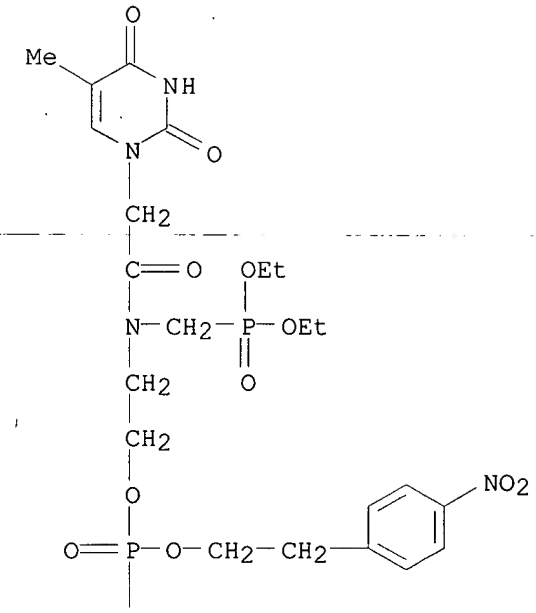
L13 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:755989 HCAPLUS
DOCUMENT NUMBER: 126:118140
TITLE: Phosphonic ester nucleic acids (PHONAs): oligodeoxyribonucleotide analog with an achiral phosphonic acid ester backbone
AUTHOR(S): Peyman, Anusch; Uhlmann, Eugen; Wagner, Konrad; Augustin, Sascha; Breipohl, Gerhard; Will, David W.; Schaefer, Andrea; Wallmeier, Holger
CORPORATE SOURCE: Hoechst AG, Frankfurt, D-65926, Germany
SOURCE: Angewandte Chemie, International Edition in English (1996), 35(22), 2636-2638
CODEN: ACIEAY; ISSN: 0570-0833
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The prepn. of polyamide nucleic acid analogs with an achiral and neg. charged backbone to which the nucleobases are attached through carboxymethylene linkers, is reported.
IT **183058-04-0P 183058-10-8P 185670-60-4P 185670-64-8P 185670-74-0P 186143-35-1P 186143-36-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of phosphonic ester nucleic acid duplexes)
RN 183058-04-0 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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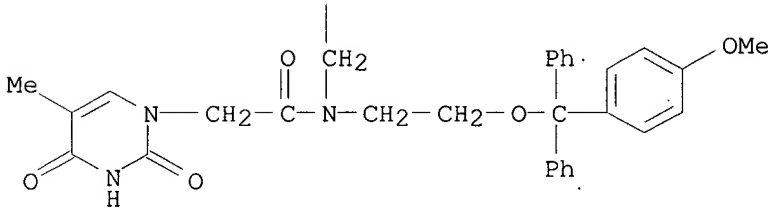
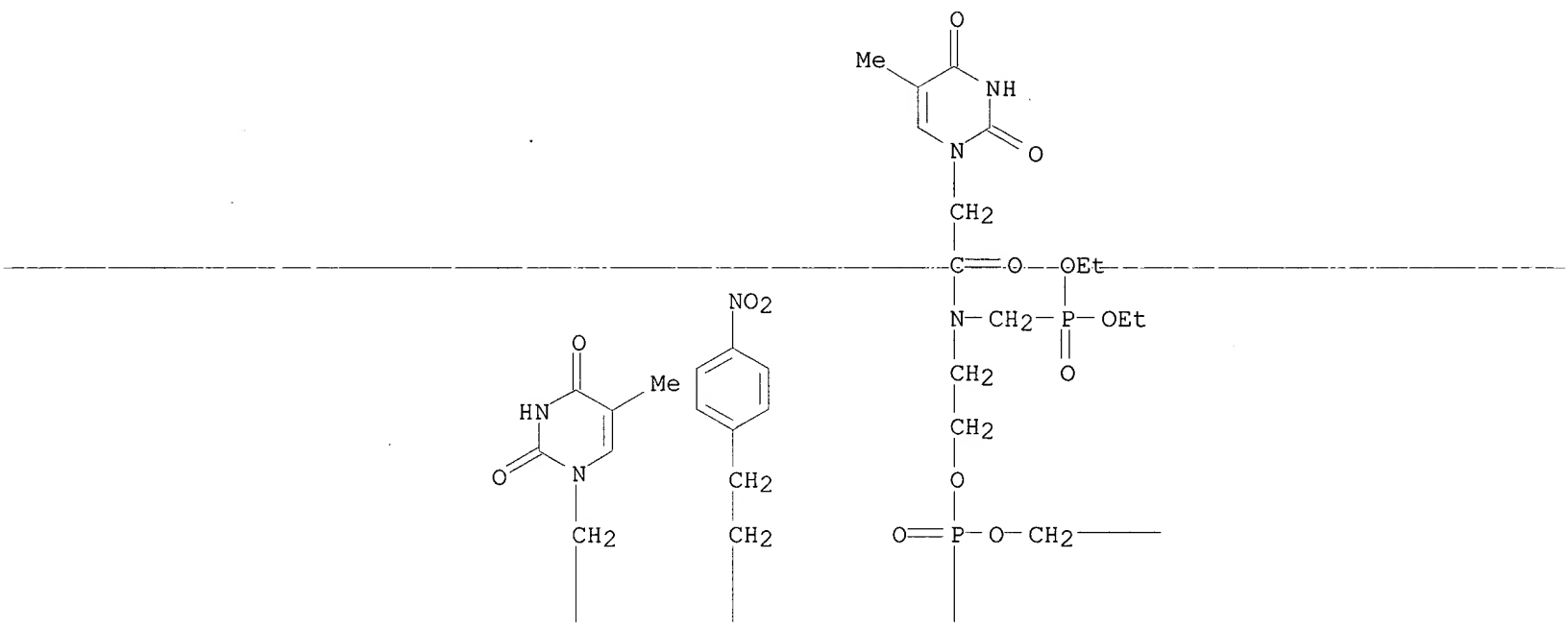


RN 183058-10-8 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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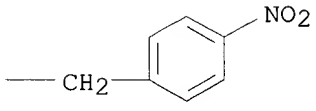

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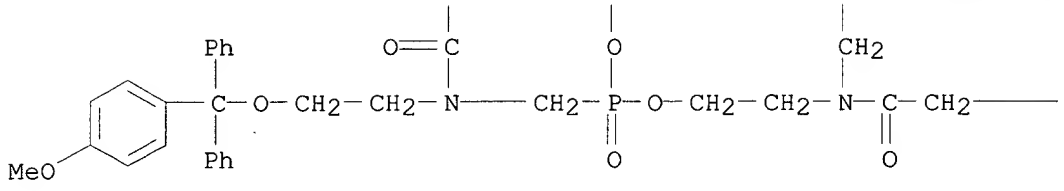

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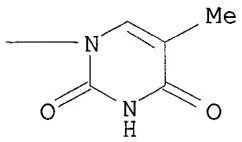
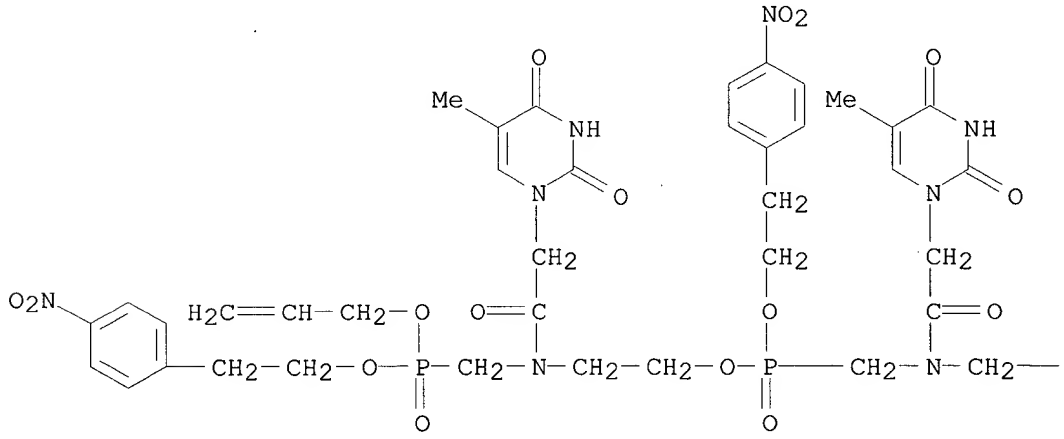


RN 185670-60-4 HCAPLUS
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-(4-nitrophenyl)ethyl 2-propenyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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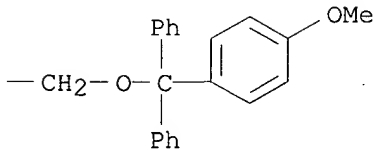
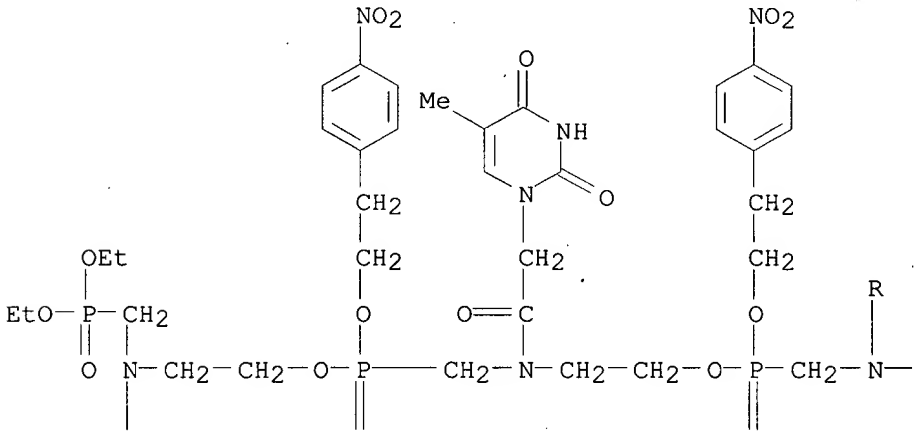


RN 185670-64-8 HCAPLUS
CN Phosphonic acid, [2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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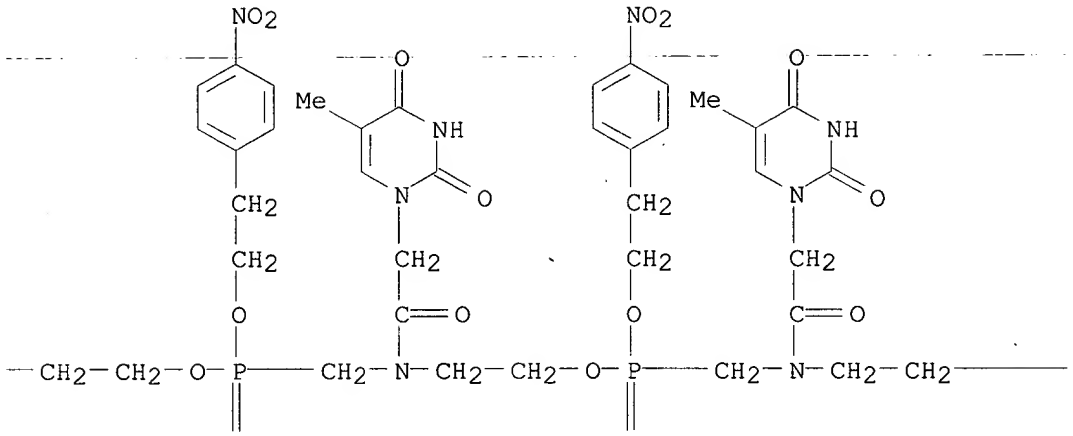

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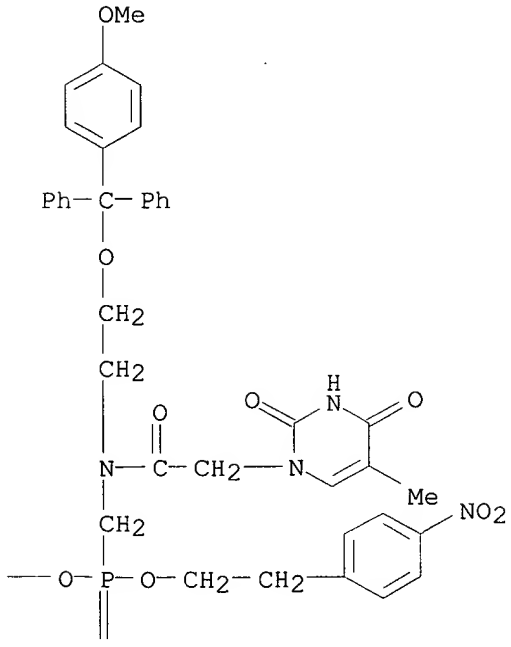

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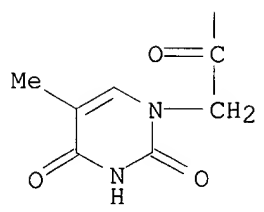

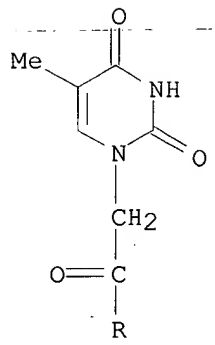

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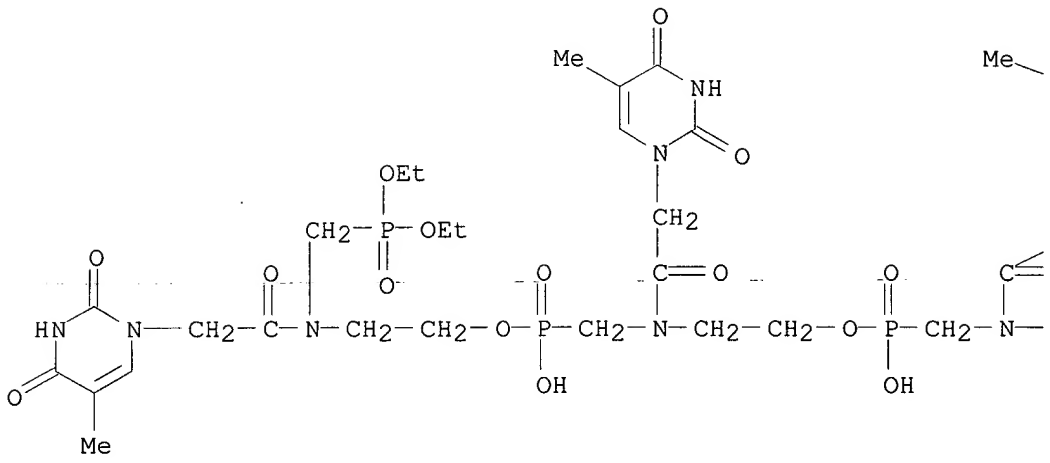
RN 185670-74-0 HCAPLUS

CN Phosphonic acid, [28-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12,18,24-tetrahydroxy-26-(2-hydroxyethyl)-6,12,18,24-tetraoxido-27-oxo-5,11,17,23-tetraoxa-2,8,14,20,26-pentaaza-6,12,18,24-tetraphosphaoctacos-1-yl]-, mono[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-23-ethoxy-5,11,17-trihydroxy-5,11,17,23-tetraoxido-6,12,18,24-tetraoxa-3,9,15,21-tetraaza-5,11,17,23-tetraphosphahexacos-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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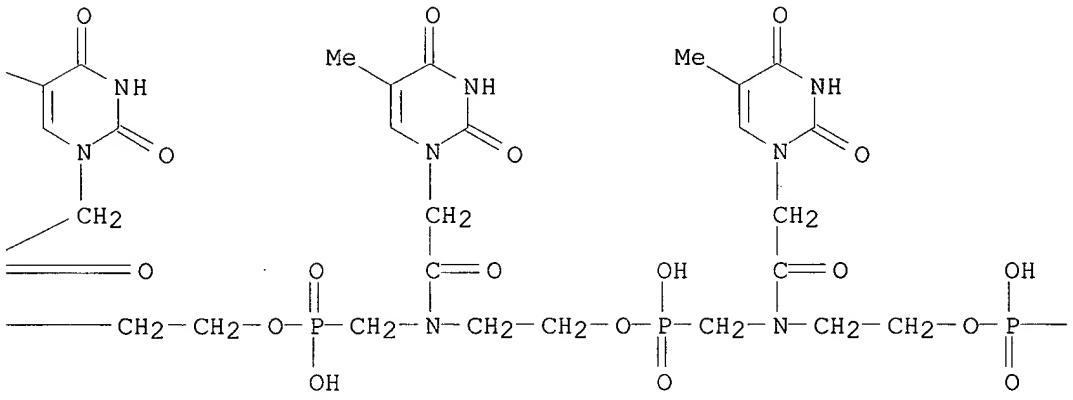

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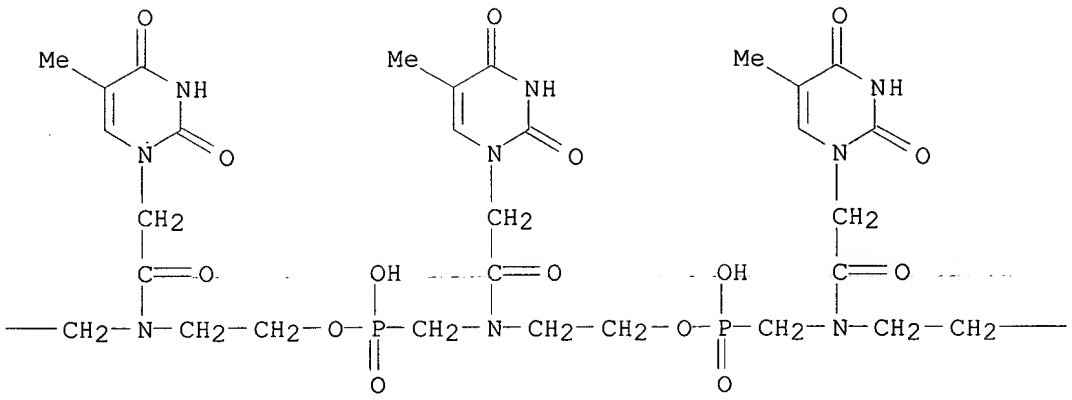

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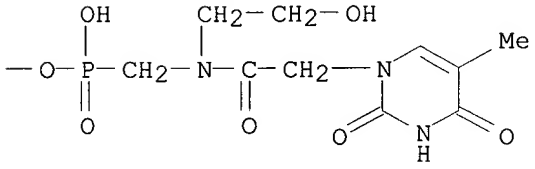

RN 186143-35-1 HCAPLUS
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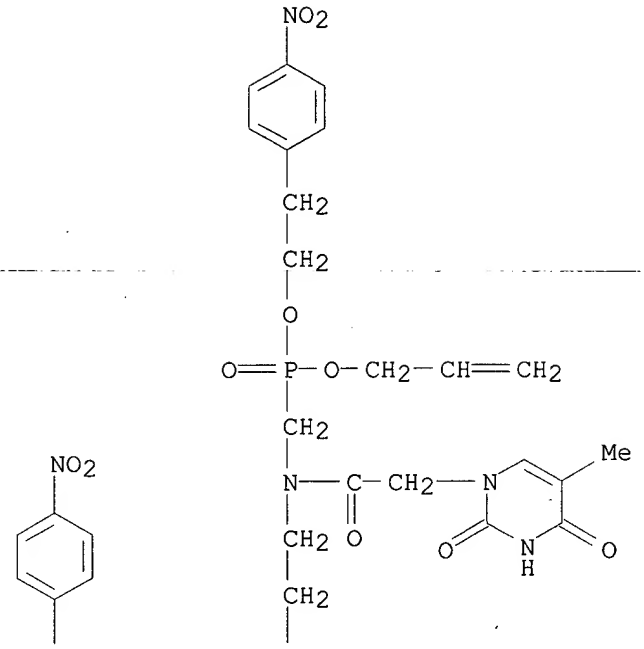
PAGE 1-A



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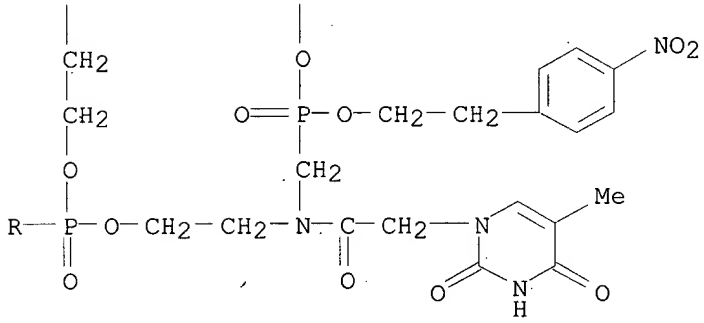

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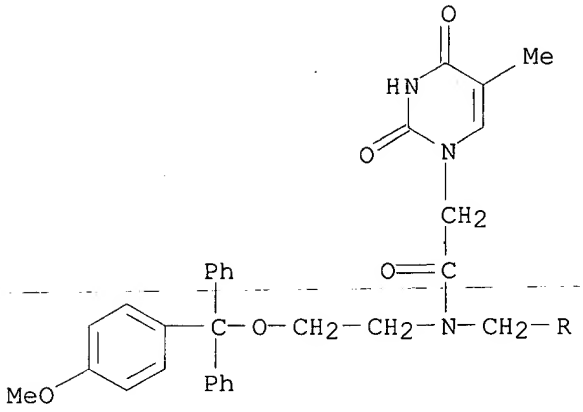

RN 186143-36-2 HCAPLUS
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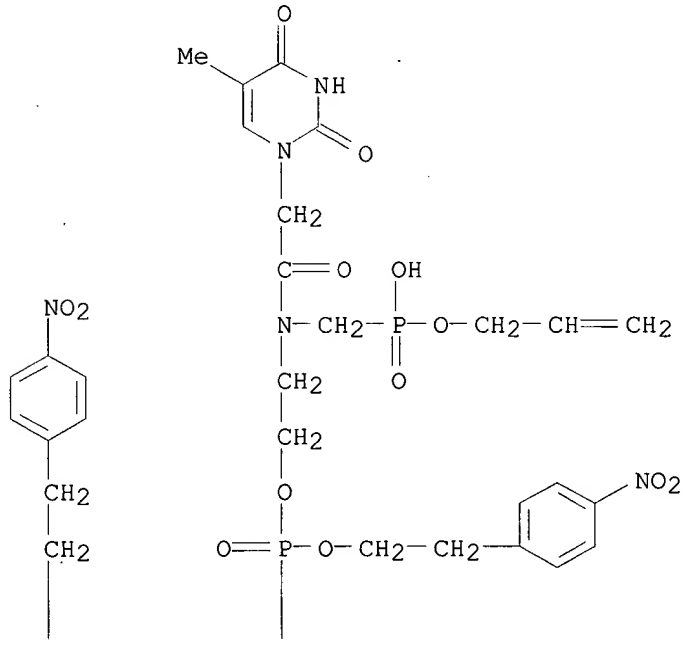
PAGE 1-A



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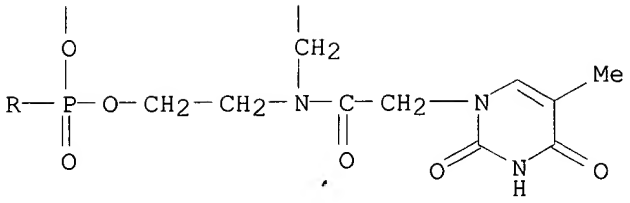

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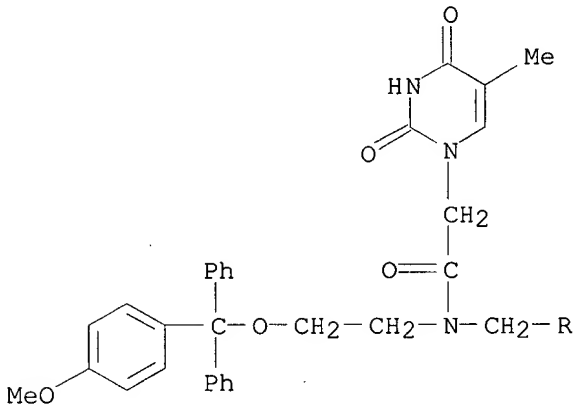

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L13 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:672510 HCAPLUS
DOCUMENT NUMBER: 125:301493
TITLE: Preparation of nucleic acid phosphonoesters as inhibitors of gene expression.
INVENTOR(S): Anuschirwan, Peyman; Uhlmann, Eugen; Breipohl, Gerhard; Wallmeier, Holger
PATENT ASSIGNEE(S): Hoechst A.-G., Germany
SOURCE: Ger. Offen., 36 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19508923	A1	19960919	DE 1995-19508923	19950313
EP 739898	A2	19961030	EP 1996-103533	19960307
EP 739898	A3	19980916		
EP 739898	B1	20010926		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 206131	E	20011015	AT 1996-103533	19960307
US 5874553	A	19990223	US 1996-613417	19960311
CA 2171589	AA	19960914	CA 1996-2171589	19960312
NO 9601006	A	19960916	NO 1996-1006	19960312
AU 9648028	A1	19960926	AU 1996-48028	19960312
AU 706470	B2	19990617		
ZA 9601986	A	19961121	ZA 1996-1986	19960312
BR 9600993	A	19971230	BR 1996-993	19960312
JP 08259579	A2	19961008	JP 1996-84808	19960313
CN 1138588	A	19961225	CN 1996-100508	19960313
CN 1060781	B	20010117		
US 6127346	A	20001003	US 1998-196132	19981120

PRIORITY APPLN. INFO.: DE 1995-19508923 A 19950313
DE 1995-19543865 A 19951124
US 1996-613417 A1 19960311

AB QXP(Z)(:Y)CR5R6L(AB)DGX[P(Z)(:Y)CR5R6L(AB)DGX]nQ1 [n = 0-100; B = H, OH, alkoxy, alkylthio, (un)natural nucleobase, reporter ligand, (substituted) alkyl, aryl, aralkyl, heterocyclyl, etc.; AB = amino acid or peptide residue; R1 = H, (substituted) alkyl; R5, R6 = H, (substituted) alkyl, aryl, aralkyl, OH, alkoxy, alkylthio; A = bond, CH2, (O-, S-, or NR1-interrupted) (substituted) alkylene; D, G = (substituted) methylene; X, Y = O, S, NR1; Z = OH, alkoxy, alkenyloxy, alkynyloxy, amino, etc.; Q, Q1 = H, conjugate, (modified) oligonucleotide], were prepd. as drugs and diagnostic agents (no data). Thus, N-(4-methoxytriphenylmethoxy)ethylamin omethanephosphonic acid di[2-(p-nitrophenyl)ethyl]ester (prepn. given) was stirred with N-ethylmorpholine, HATU, and N6-anisoylcytosine-1-acetic acid in DMF to give a coupling product which was stirred with DBU in MeCN to give N-(N6-anisoylcytosin-1-ylacetyl)-N-(4-methoxytriphenylmethoxy)ethylam inomethanephosphonic acid [2-(p-nitrophenyl)ethyl] monoester.

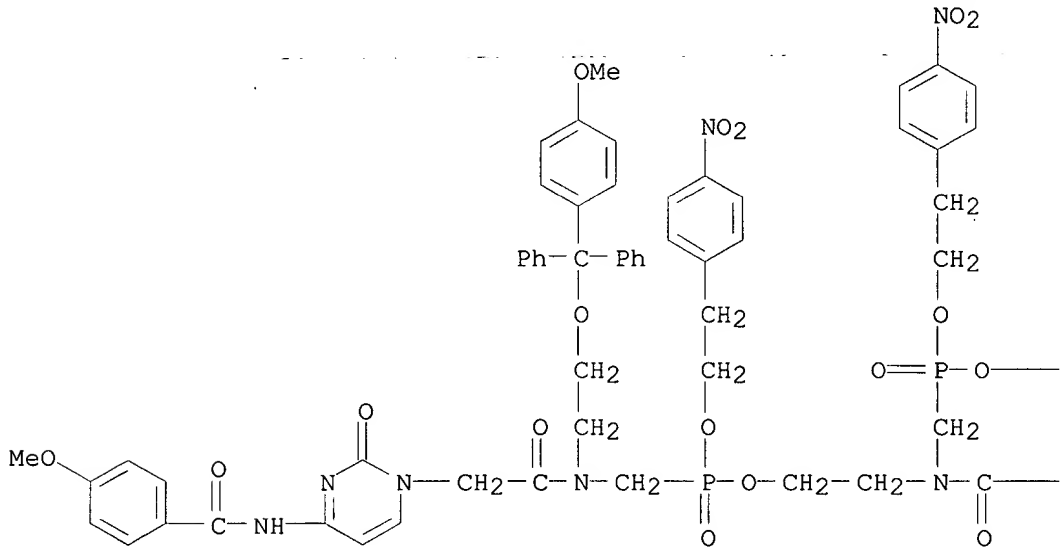
IT **183057-63-8P 183057-66-1P 183057-94-5P**
183058-06-2P 183058-10-8P 183058-11-9P
183058-12-0P 183058-14-2P
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of nucleic acid phosphonoesters as inhibitors of gene expression)

RN 183057-63-8 HCAPLUS

CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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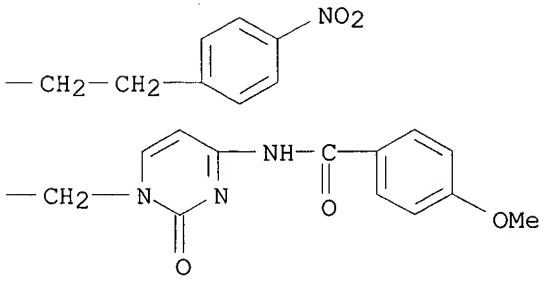

RN 183057-66-1 HCAPLUS

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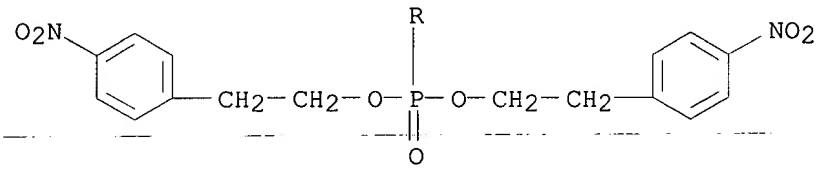
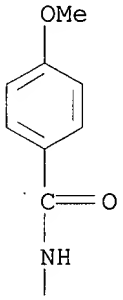
PAGE 1-A





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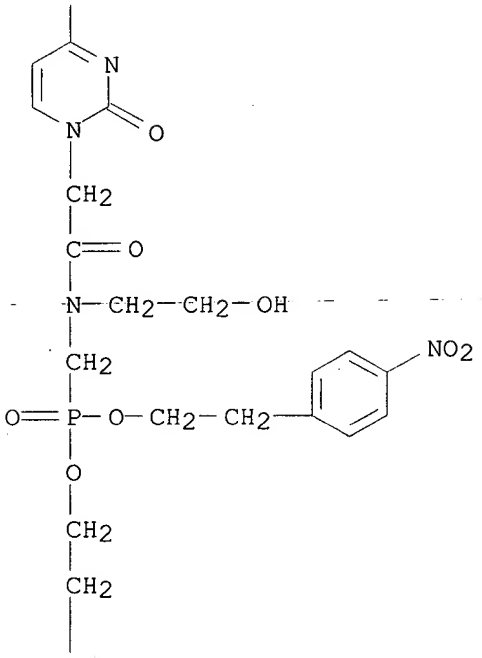

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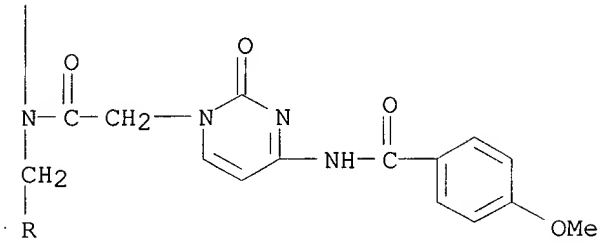

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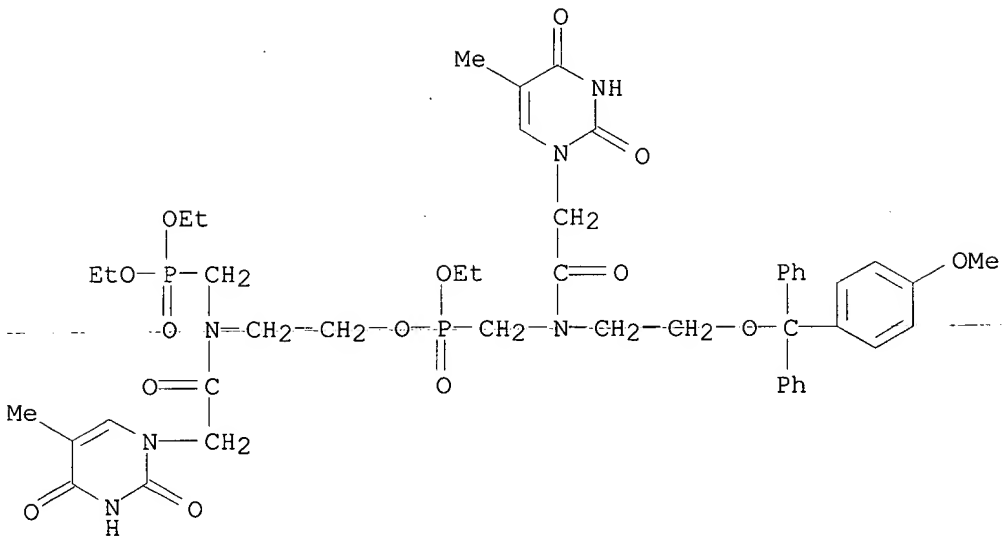
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6-ethoxy-12-(4-methoxyphenyl)-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



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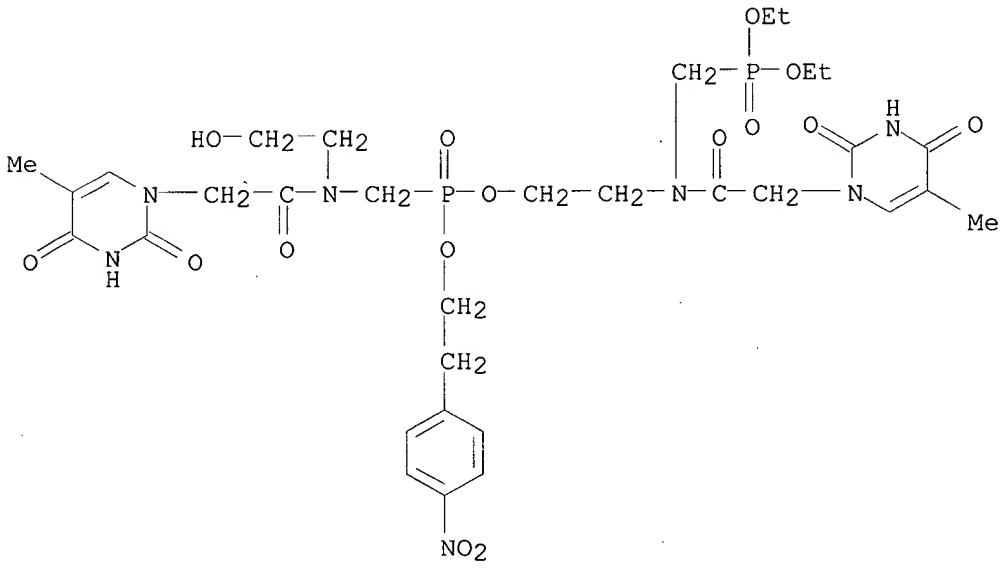
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



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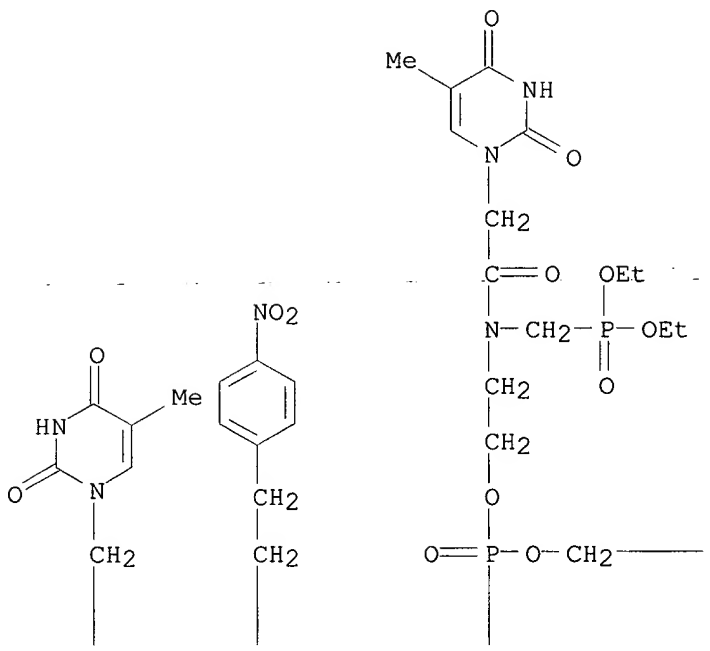
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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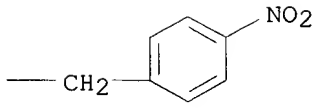

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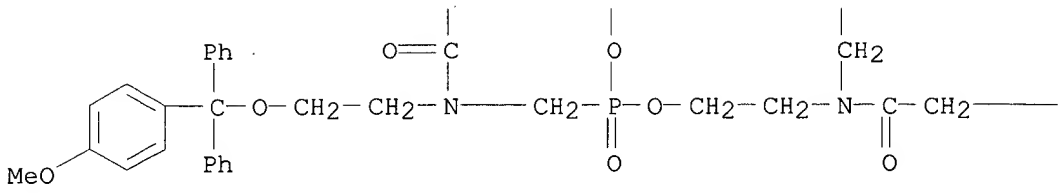

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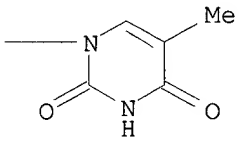

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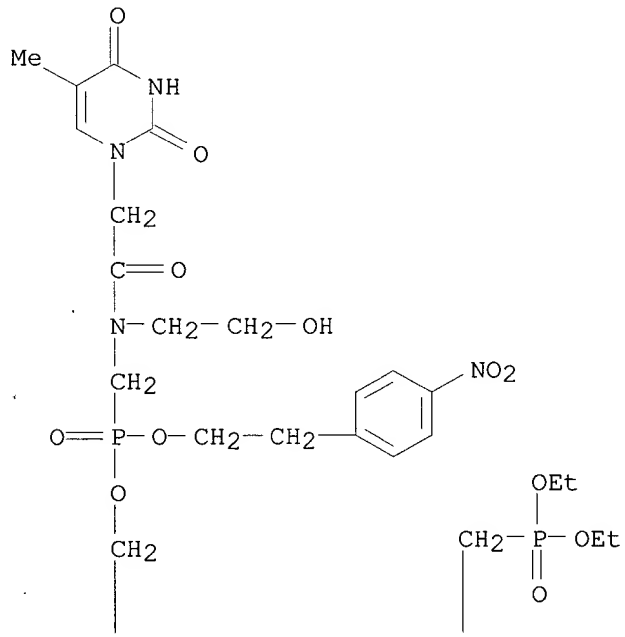
PAGE 1-A



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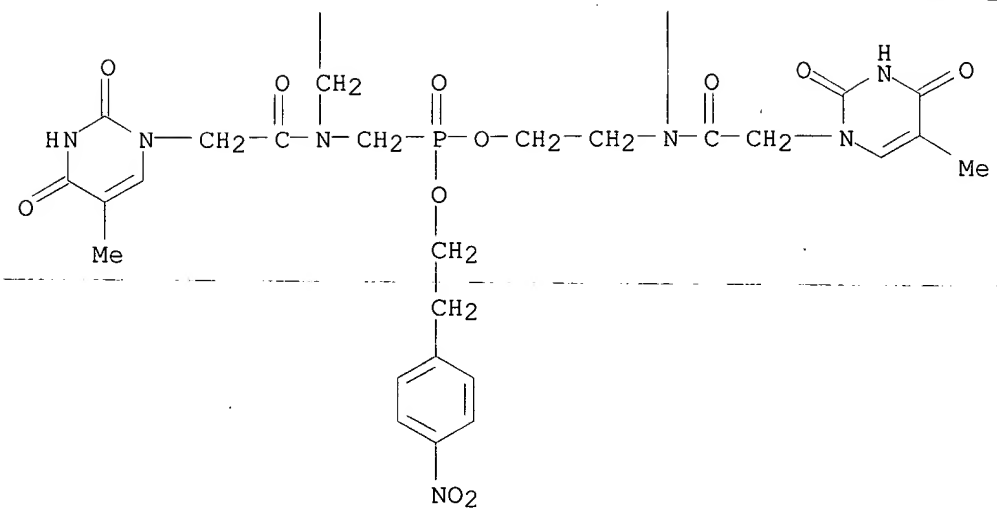

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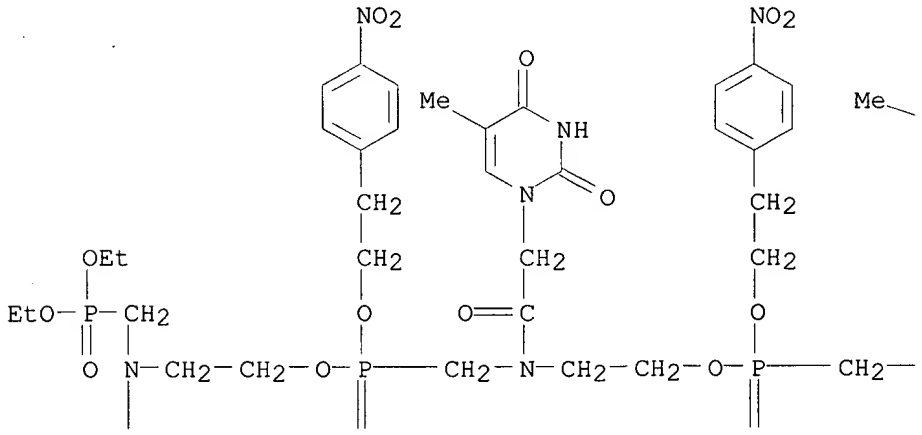

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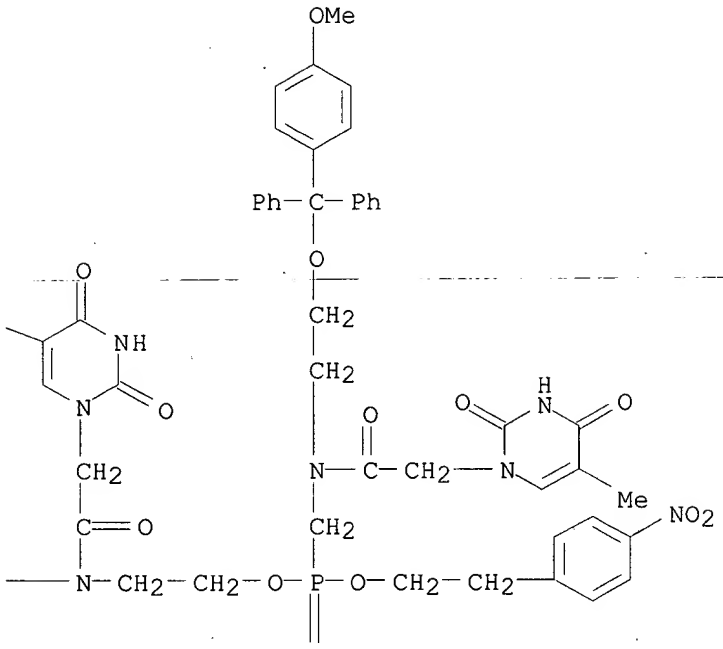

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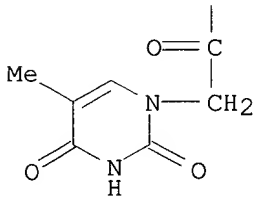

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CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

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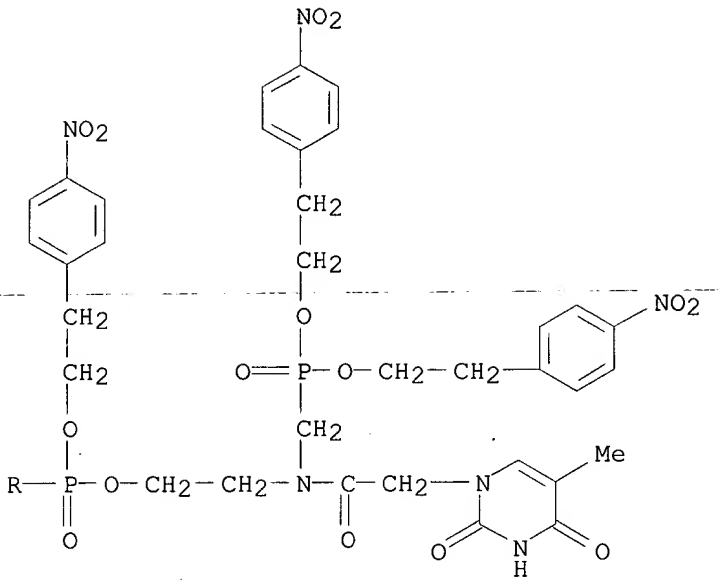

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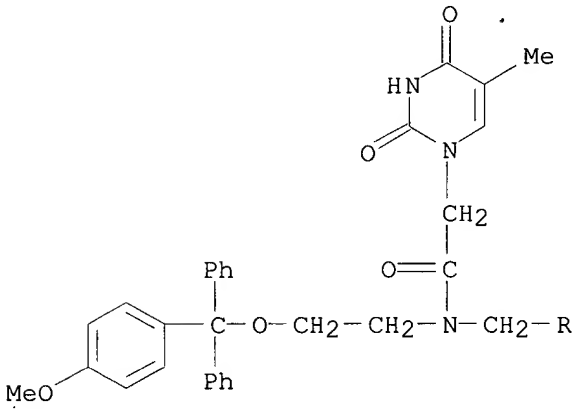
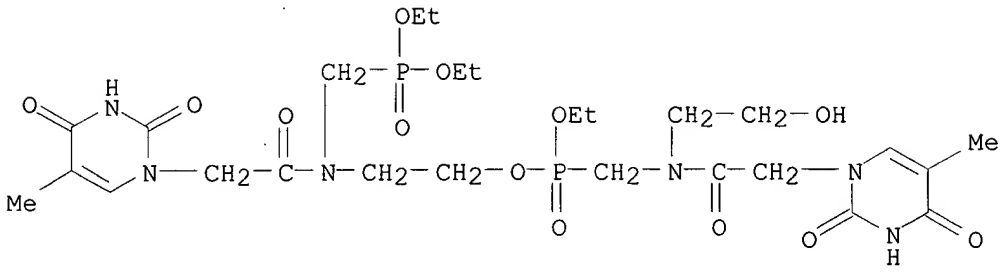


IT **183057-96-7P 183057-99-0P 183058-04-0P**
183058-09-5P 183058-13-1P 183058-15-3P
183058-16-4P 183058-18-6P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nucleic acid phosphonoesters as inhibitors of gene expression)

RN 183057-96-7 HCAPLUS

CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl ethyl ester (9CI) (CA INDEX NAME)



RN 183057-99-0 HCAPLUS
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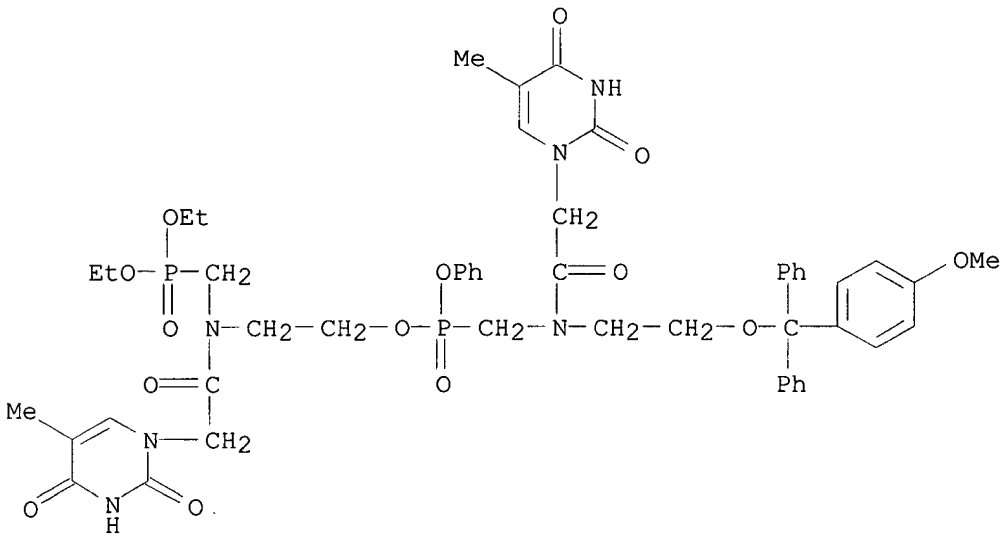

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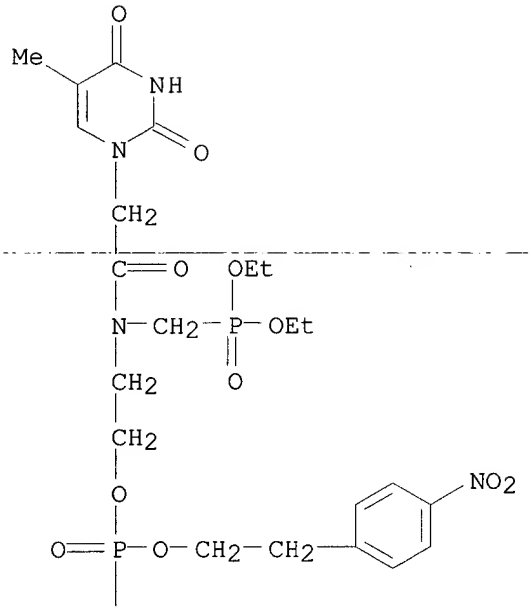
PAGE 1-A



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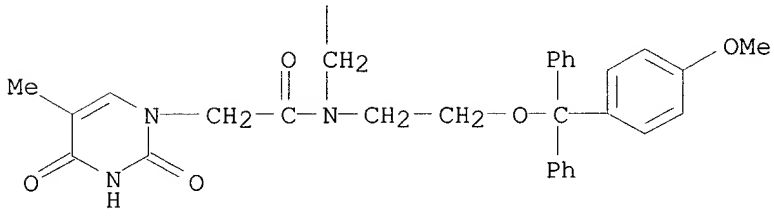

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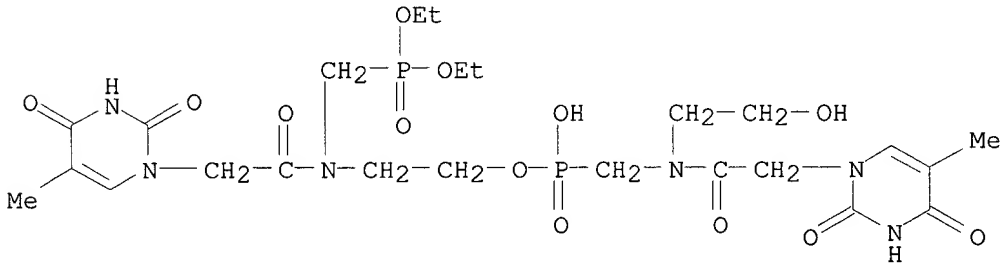

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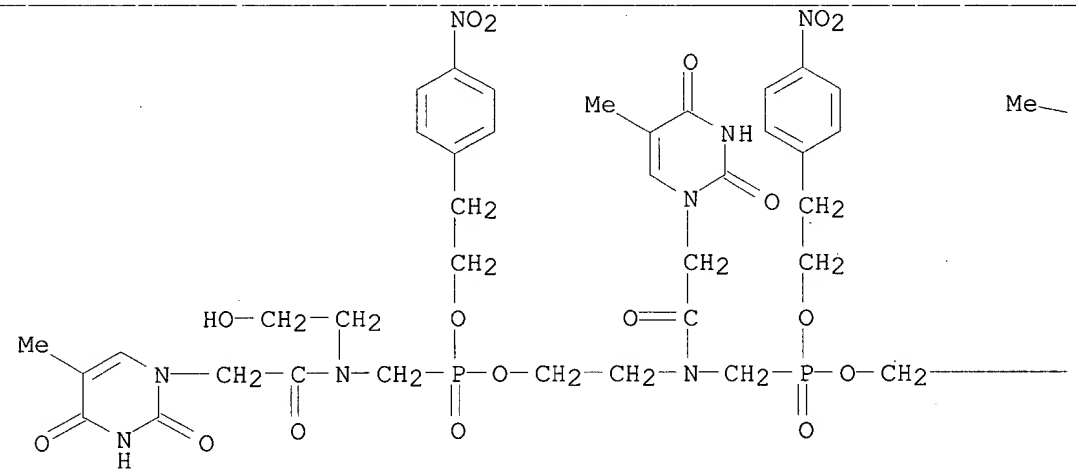

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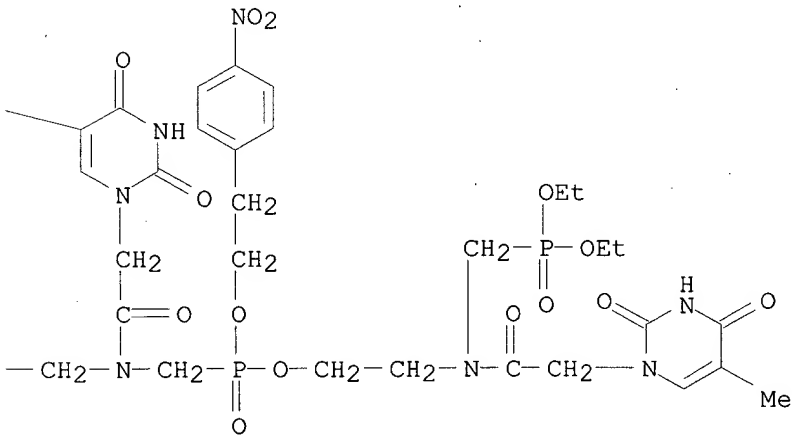

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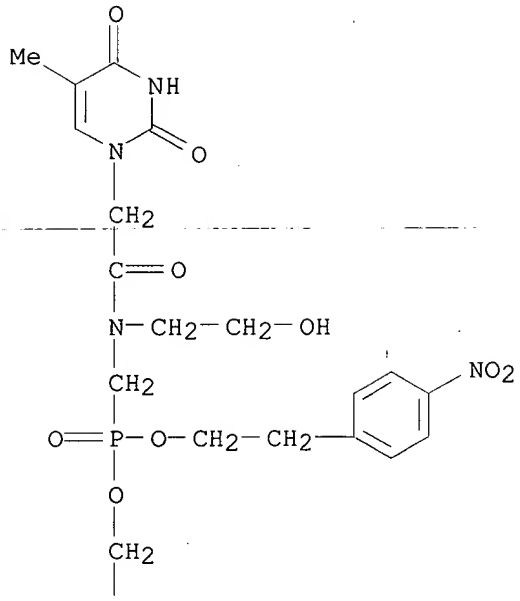

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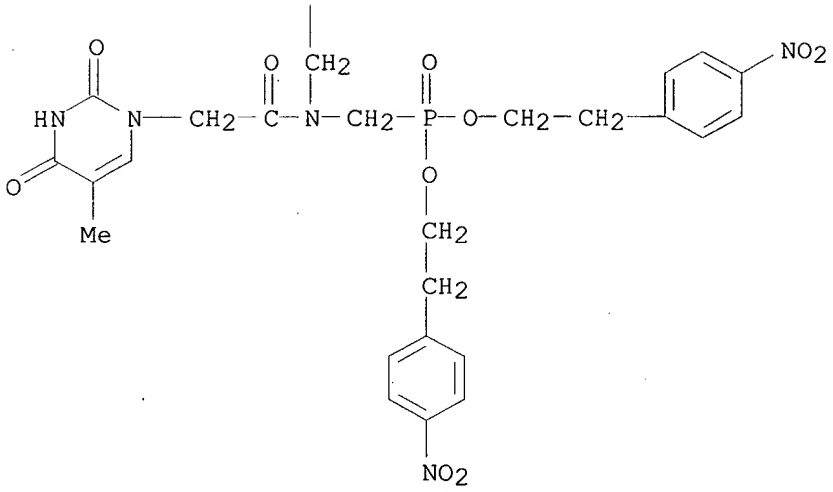
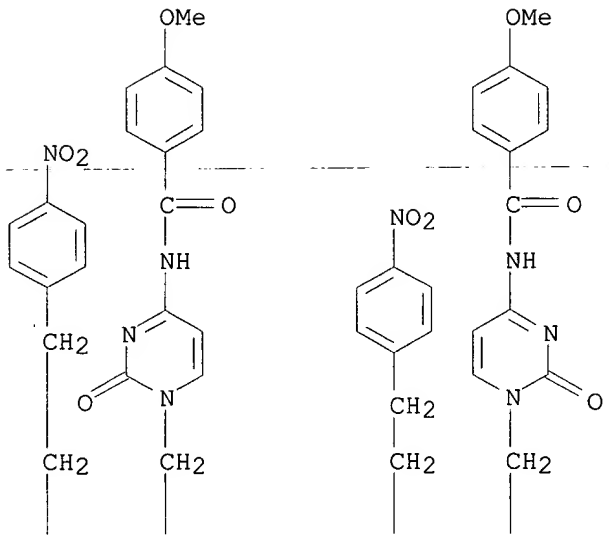


RN 183058-16-4 HCAPLUS
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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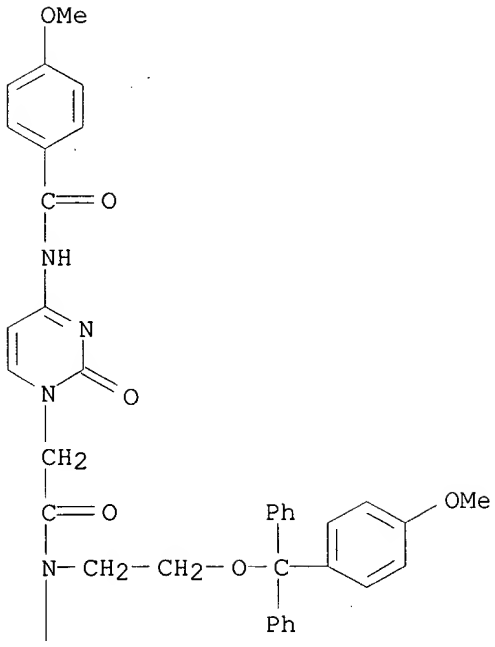

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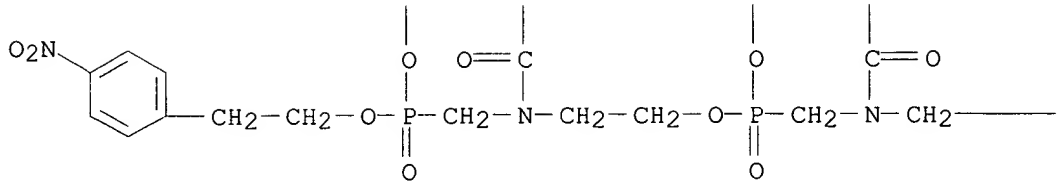

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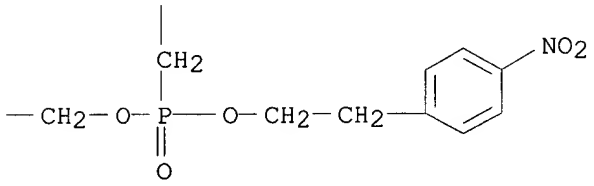
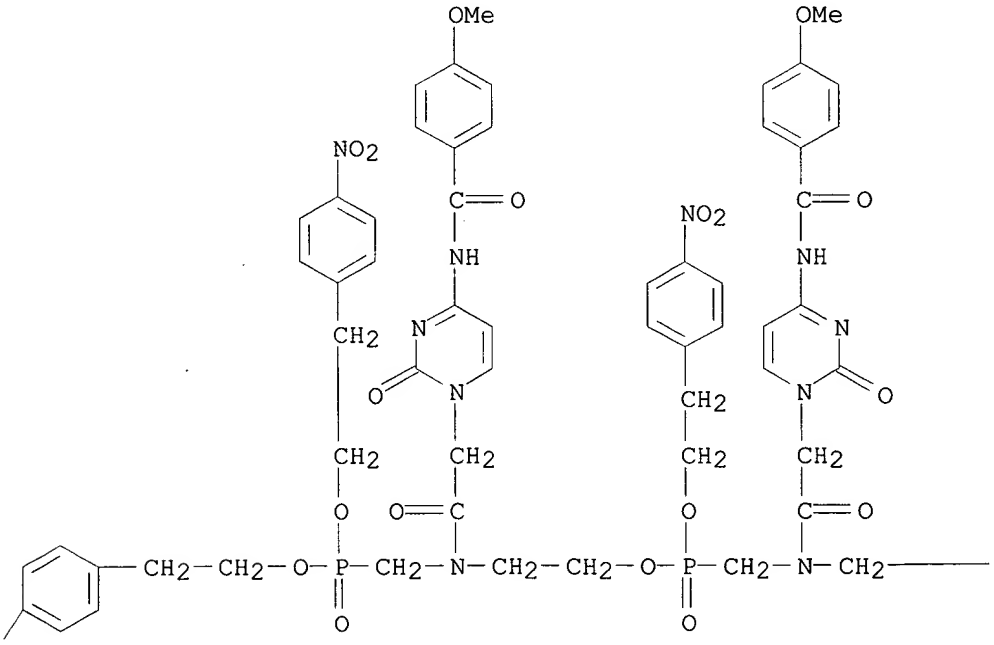


RN 183058-18-6 HCAPLUS
CN Phosphonic acid, [8-(2-hydroxyethyl)-10-[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]-2-[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-9-oxo-5-oxa-2,8-diaza-6-phosphadec-1-yl]-, 2-[[[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

PAGE 1-A



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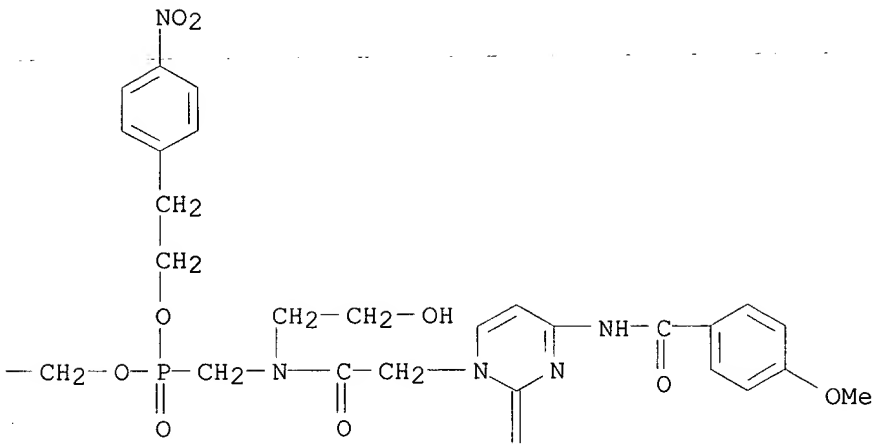


PAGE 2-A

PAGE 2-B

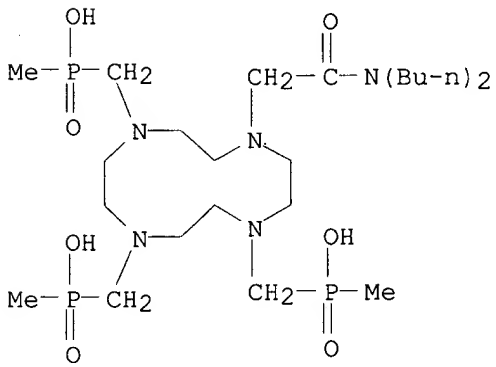
=> d ibib abs hitstr 11

L13 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:55156 HCAPLUS
DOCUMENT NUMBER: 124:218502
TITLE: Extent of hydration of octadentate lanthanide complexes incorporating phosphinate donors: solution relaxometry and luminescence studies
AUTHOR(S): Aime, Silvio; Botta, Mauro; Parker, David; Williams, J. A. Gareth
CORPORATE SOURCE: Dip. Chim. Inorg., Univ. Torino, Turin, 10125, Italy
SOURCE: J. Chem. Soc., Dalton Trans. (1996), (1), 17-23
CODEN: JCDTBI; ISSN: 0300-9246
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The behavior of luminescent (Eu, Tb) and highly paramagnetic (Gd) complexes of 1,4,7,10-tetraazacyclododecane contg. one carboxamide and three phosphinate substituents was studied in soln. Anal. of variable-temp. nuclear magnetic relaxation dispersion profiles indicate that there is no H2O mol. directly coordinated to Gd(III) ions. The obsd. relaxation enhancement of solvent protons is detd., in addn. to the contribution from H2O mols. diffusing in close proximity to the paramagnetic complex, by a relatively distant H2O mol. in the 'second coordination sphere'. This is possible because the amide carbonyl O can participate in H bonding (as a H-bond acceptor) to a local H2O mol., which brings the H2O mol. close to the metal ion. The luminescence spectra of the complexes of Eu and Tb in H2O and D2O are also consistent with such a hydration scheme and there is a good correlation between the nonintegral q value (no. of inner-sphere H2O mols.) detd. by this method and the distance between the metal ion and the H2O proton estd. by relaxometric methods. Probably the hydration states q = 0 and 1 may be considered to represent boundary conditions and a given complex in soln. may possess intermediate values.

IT **145130-40-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(extent of hydration of octadentate lanthanide complexes incorporating phosphinate donors studied by soln. relaxometry and luminescence)

RN 145130-40-1 HCAPLUS
CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 12

L13 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:881296 HCAPLUS
DOCUMENT NUMBER: 123:286533
TITLE: Preparation of reagents comprising chimeric molecules of nucleic acids and nucleic acid analogs as primers
INVENTOR(S): Reeve, Michael Alan; Brown, Tom
PATENT ASSIGNEE(S): Amersham International PLC, UK
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9508556	A1	19950330	WO 1994-GB2053	19940921
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9476617	A1	19950410	AU 1994-76617	19940921
EP 720615	A1	19960710	EP 1994-927002	19940921
EP 720615	B1	20000726		
R: DE, DK, FR, GB, IT, SE				
US 2002068275	A1	20020606	US 1996-617781	19960521

PRIORITY APPLN. INFO.: EP 1993-307455 A 19930921
WO 1994-GB2053 W 19940921

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Chimeric mols. of nucleic acid/nucleic acid analog, comprising a nonstandard backboned oligonucleotide having at least one amide linkage and a std. backboned portion having a 3' acceptor end which is a chem. functionality capable of acting as an acceptor for the formation of a phosphodiester bond, useful as primers in reactions involving primer extension, such as nucleic acid amplification and sequencing, are prepd. A method for performing a primer extension reaction comprises mixing (a) a target nucleic acid (preferably a double-stranded nucleic acid), (b) a primer which is the said chimeric mol. capable of hybridizing to part of the target, and (c) a supply of nucleotides in the presence of a chain extension enzyme under conditions to allow the chimeric mol. to hybridize to the target and extension of the chimeric mol. at the acceptor end to occur and to give an extension product. A method for performing a chain termination reaction comprises mixing reagents a, b, and c (wherein preferably at least one of the reagents is labeled) in the presence of a chain extension enzyme under conditions to allow the chimeric mol. to hybridize to the target and extension of the chimeric mol. at the acceptor end to occur and to produce terminated extension products which are sepd. to allow part of the nucleotide sequence of the target nucleic acid to be detd. A method for detg. the nucleotide sequence of a target nucleic acid

comprises performing the latter method using a chain termination agent for each of the four different nucleotides such that the nucleotide sequence of the target may be detd. Thus, a peptide/oligonucleotide mol. (I) was prepd. by the solid phase method using std. phosphoramidite chem., a Applied Biosystems DNA synthesizer model 394, and intermediates Et N-(monomethoxytritylaminoethyl)-N-(thyminylacetyl)glycinate (II) (prepn. given) and 5'-amino-5'-deoxythymidine deriv. (III) (prepn. given). In primer extension assay using Klenow or exonuclease free Klenow, I gave efficient priming of the 18-mer DNA template 5'-CTGAACAACACTCTAAAA-3.

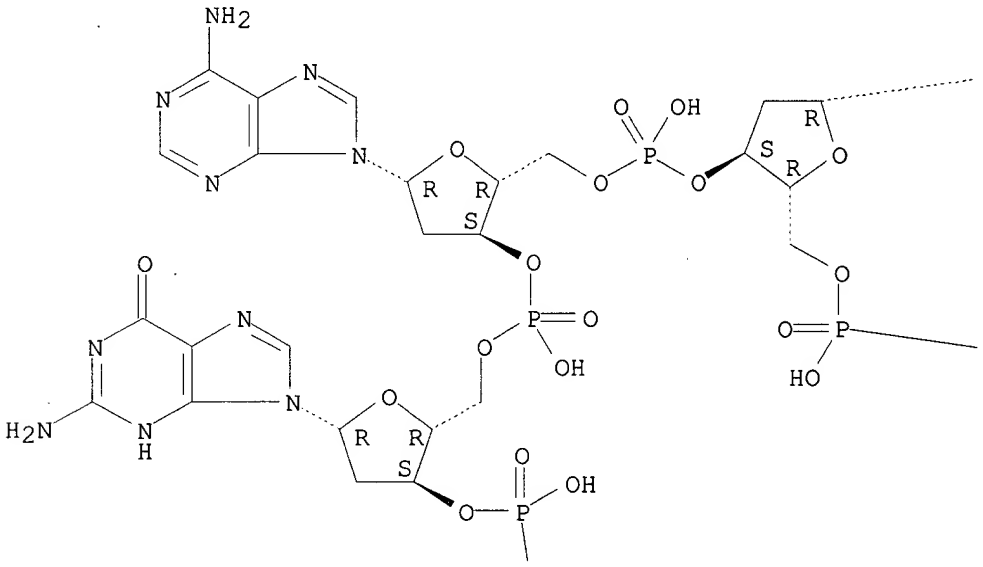
IT **169452-42-0P 169452-43-1P**
RL: ARG (Analytical reagent use); BPR (Biological process); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)
(prepn. of chimeric peptide/nucleic acid analogs contg. amide bonds as primers for DNA sequencing and amplification)

RN 169452-42-0 HCAPLUS

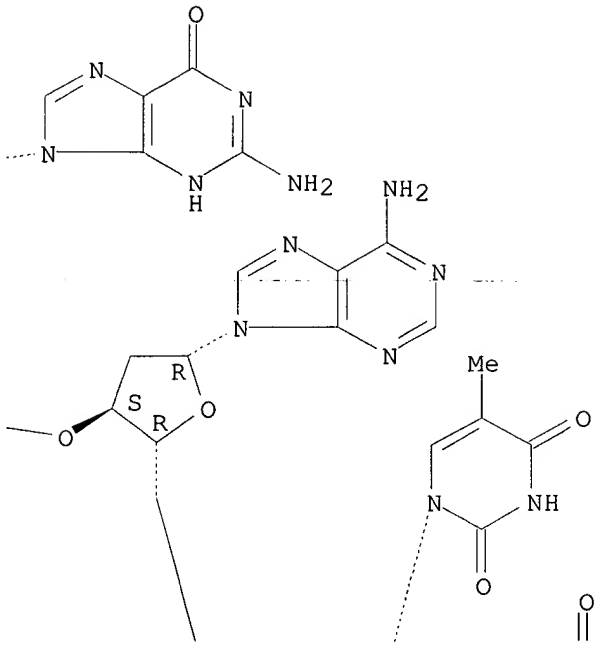
CN Thymidine, 5'-[[17-amino-3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13-trioxo-3,6,9,12,15-pentaazaheptadec-1-yl]amino]-5'-deoxythymidylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

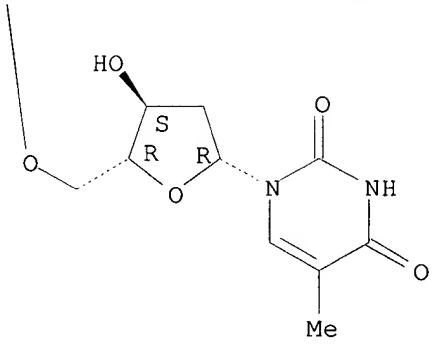
PAGE 1-A



PAGE 1-B



PAGE 2-A



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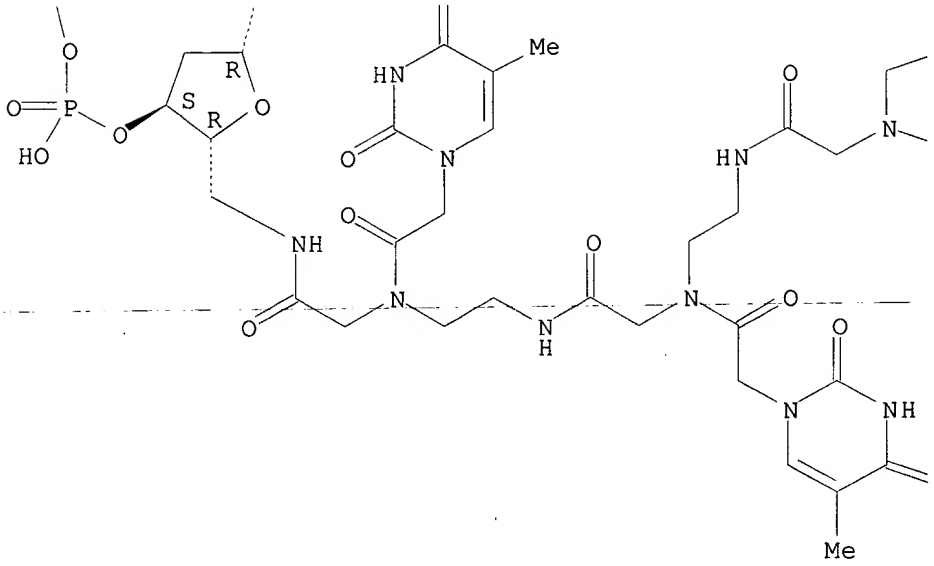

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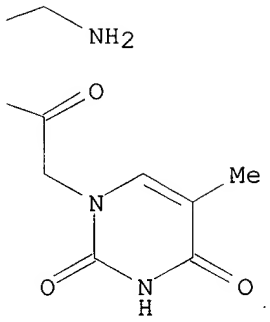
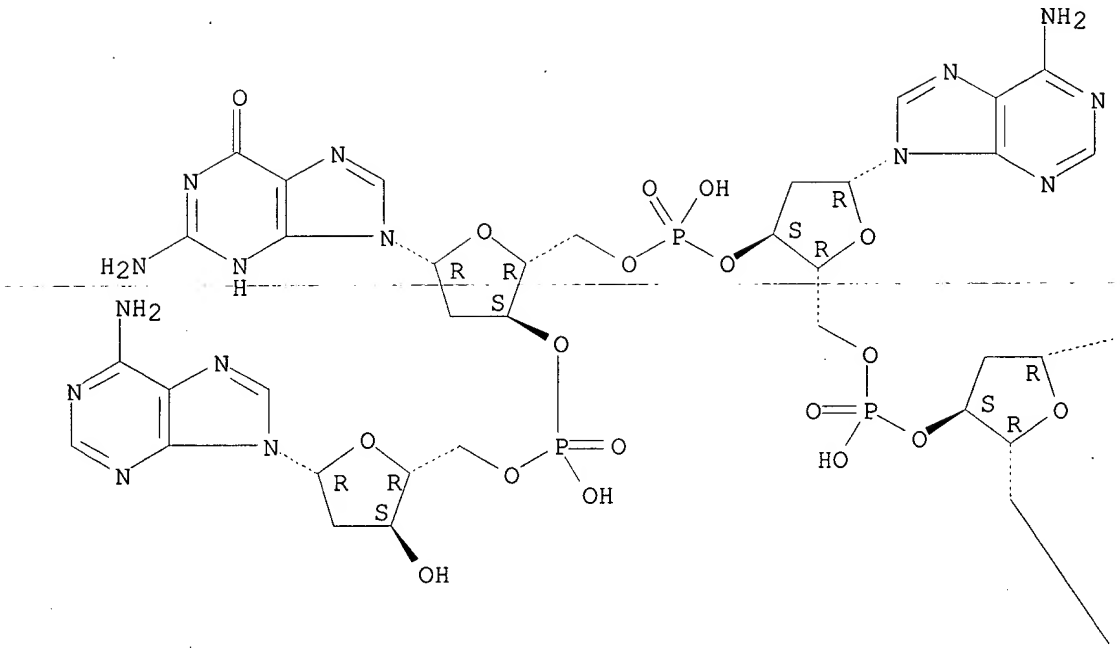


RN 169452-43-1 HCAPLUS

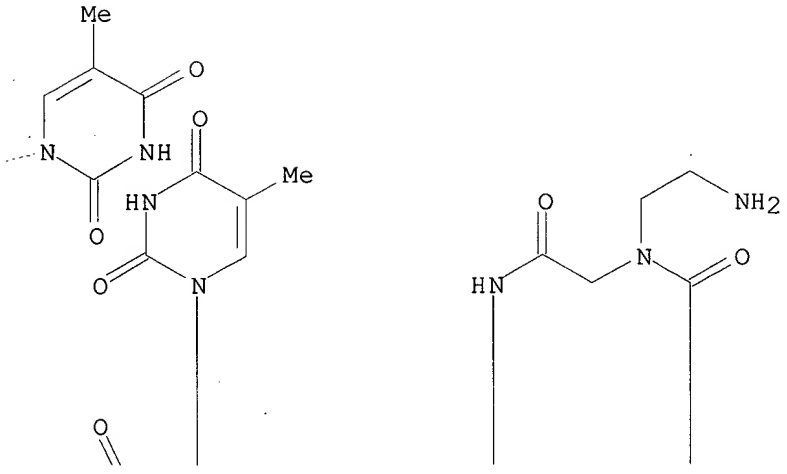
CN Adenosine, 5'-[[17-amino-3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13-trioxo-3,6,9,12,15-pentaazaheptadec-1-yl]amino]-5'-deoxythymidylyl-(3'.fwdarw.5')-2'-deoxyadenylyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



PAGE 2-A

O

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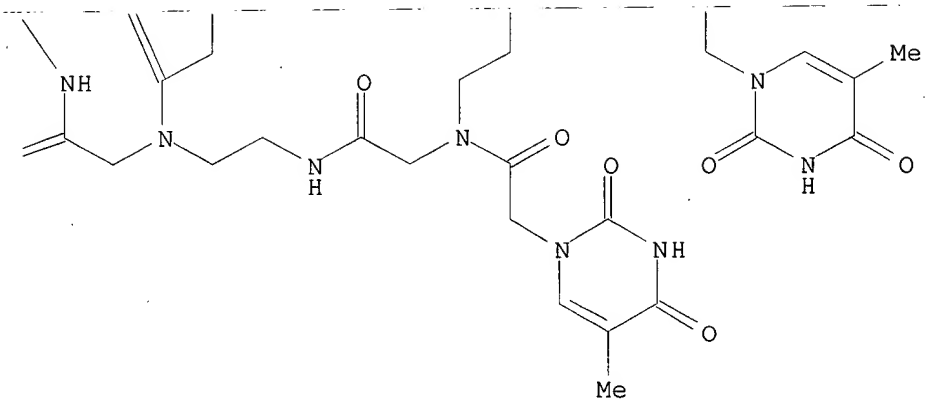
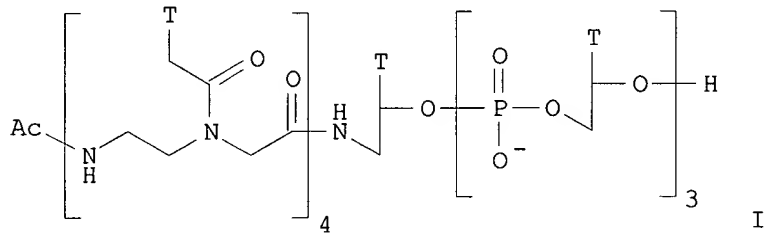


=> d ibib abs hitstr 13

L13 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1995:752363 HCAPLUS
DOCUMENT NUMBER: 124:9293
TITLE: Solid support synthesis of a PNA-DNA hybrid
AUTHOR(S): van der Laan, A. C.; Meeuwenoord, N. J.; Kuyl-Yeheskiely, E.; Oosting, R. S.; Brands, R.; van Boom, J. H.
CORPORATE SOURCE: Leiden Inst. Chem., Leiden Univ., Leiden, 2300 RA, Neth.
SOURCE: Recl. Trav. Chim. Pays-Bas (1995), 114(6), 295-7
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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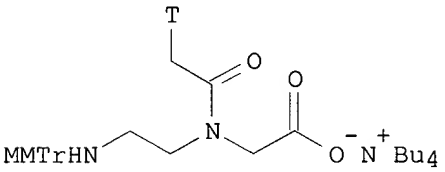

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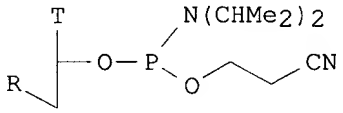


III

AB The solid support synthesis of a homothymine peptide nucleic acid (PNA)-DNA octamer (i.e. hybrid I; T = thymin-1-yl), which is an antisense oligonucleotide analog (no data), could be realized using tetrabutylammonium N-[2-(4-methoxytrityl)aminoethyl]-N-[(thymin-1-yl)acetyl]glycinate (II) as PNA building block and the resp. 2-cyanoethyl-N,N-diisopropylphosphoramidite derivs. of both 5'-O-(4,4'-dimethoxytrityl)thymidine and 5'-N-(4-methoxytrityl)amino-5'-deoxythymidine (III; R = O-DMTr, NH-MMTr).

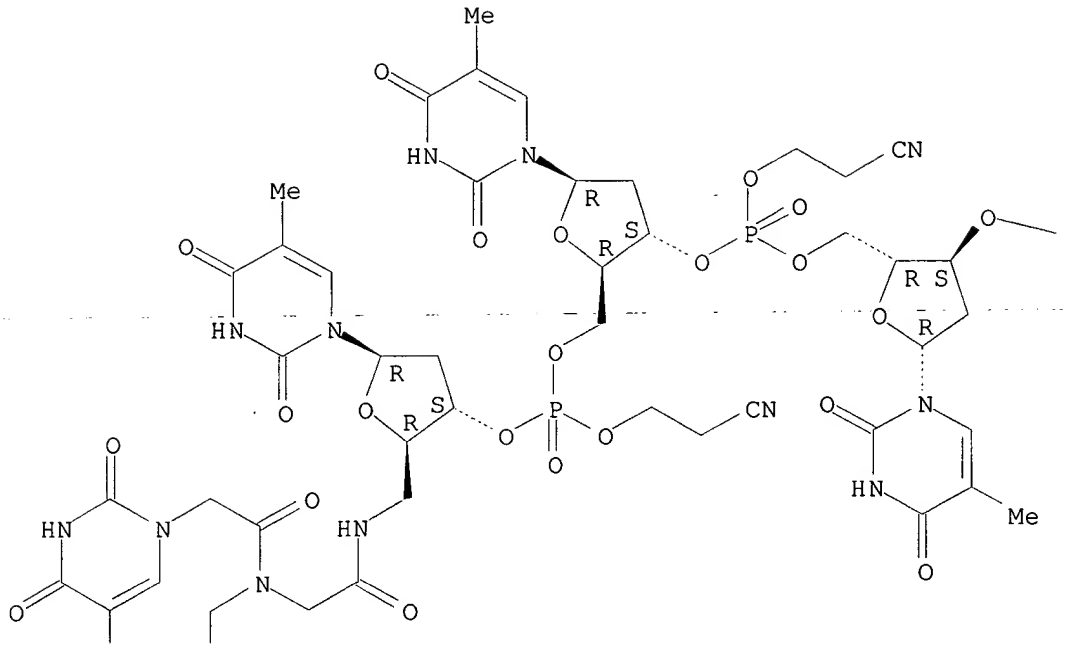
IT **170944-01-1DP**, support-bound **170944-02-2DP**, support-bound **170944-03-3DP**, support-bound
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(solid support synthesis of homothymine peptide nucleic acid-DNA hybrid as antisense oligonucleotide analog)

RN 170944-01-1 HCAPLUS

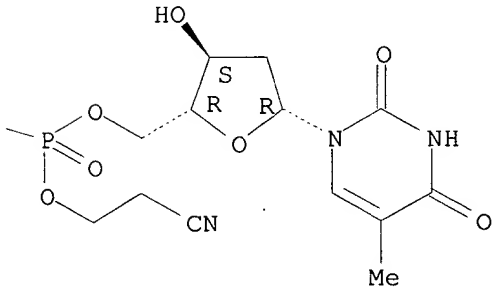
CN Thymidine, P-(2-cyanoethyl)-5'-deoxy-5'-[[[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl][2-[[(4-methoxyphenyl)diphenylmethyl]amino]ethyl]amino]acetyl]amino]thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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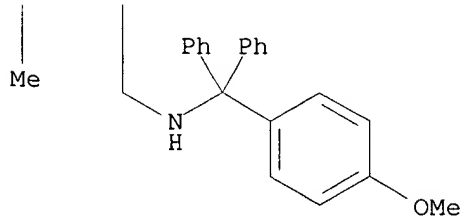
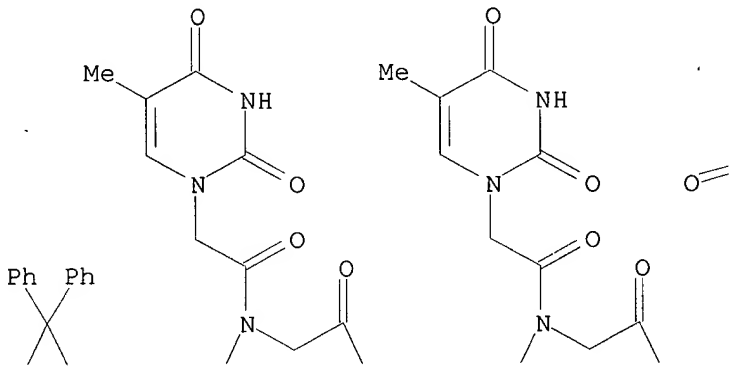


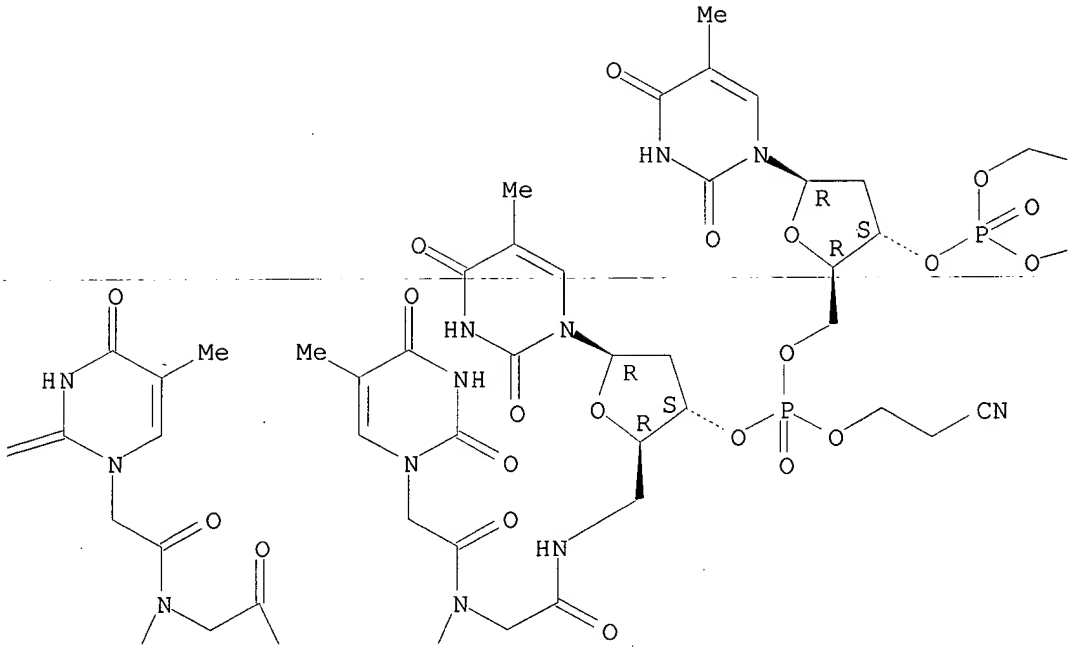
RN 170944-02-2 HCAPLUS
CN Thymidine, P-(2-cyanoethyl)-5'-deoxy-5'-[[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-25-(4-methoxyphenyl)-1,7,13,19-tetraoxo-25,25-diphenyl-3,6,9,12,15,18,21,24-octaazapentacos-1-yl]amino]thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



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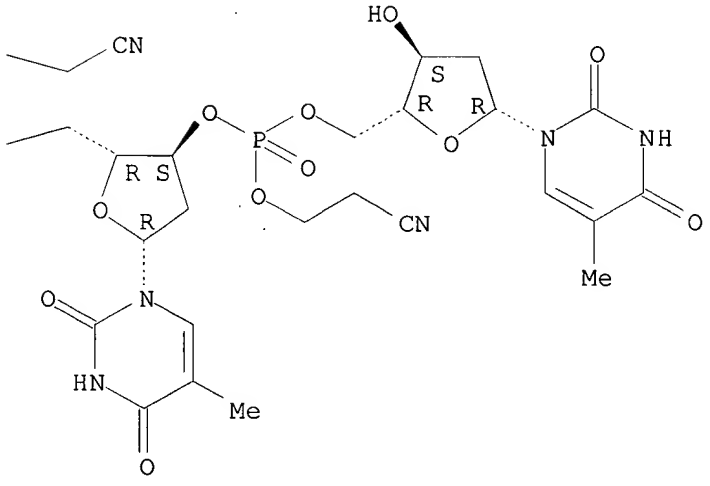

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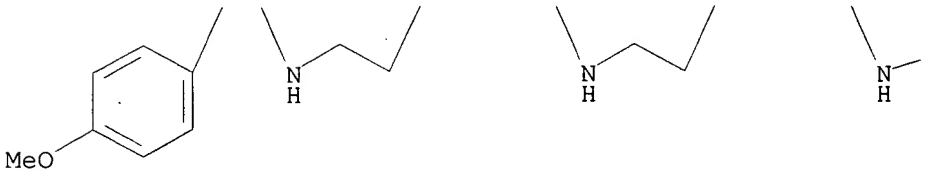

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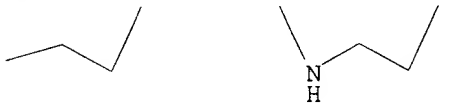

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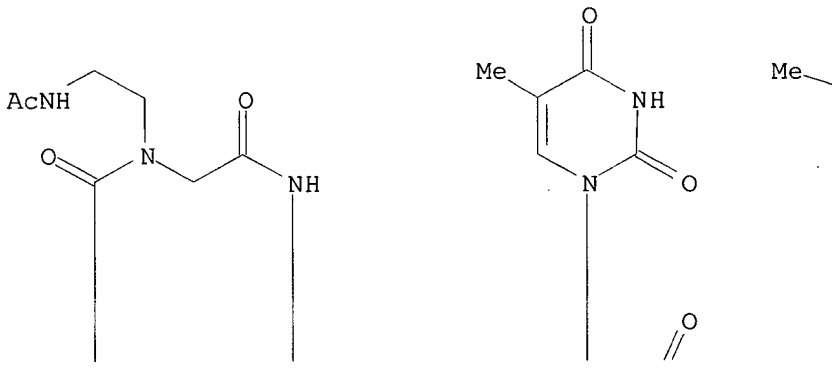
CN Thymidine, P-(2-cyanoethyl)-5'-deoxy-5'-[[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13,19,25-pentaoxo-3,6,9,12,15,18,21,24-octaazahexacos-1-yl]amino]thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



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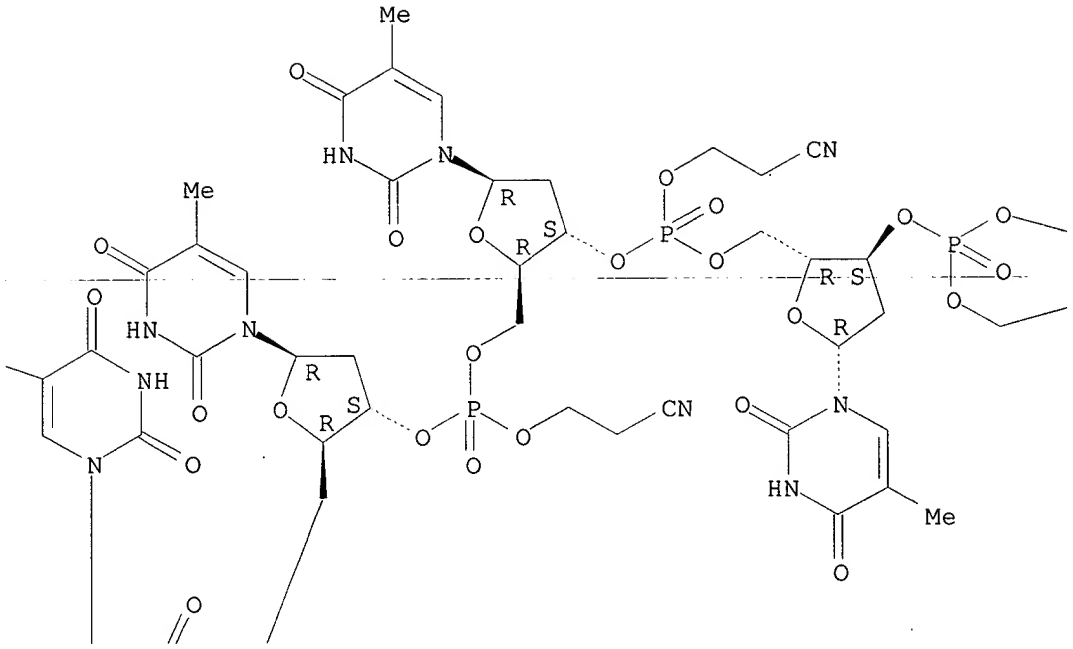

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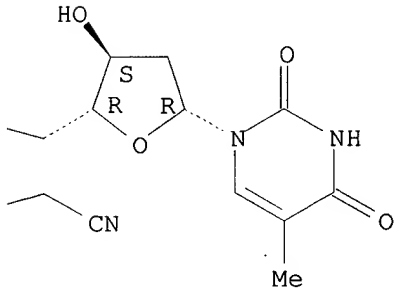
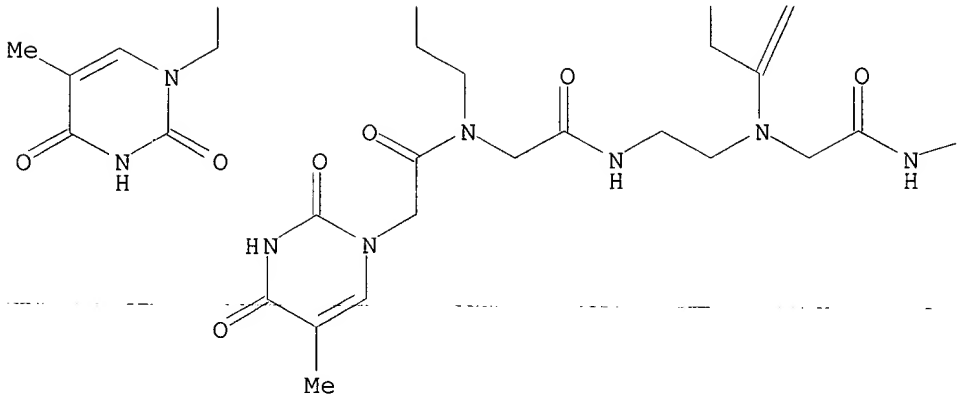


PAGE 2-A



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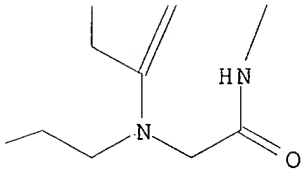
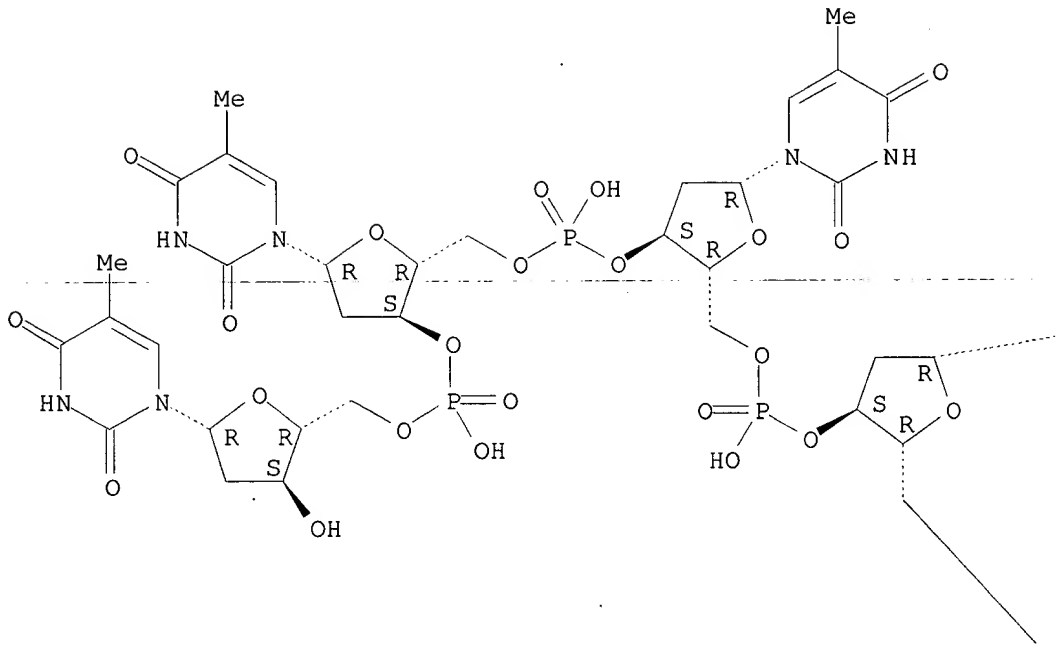


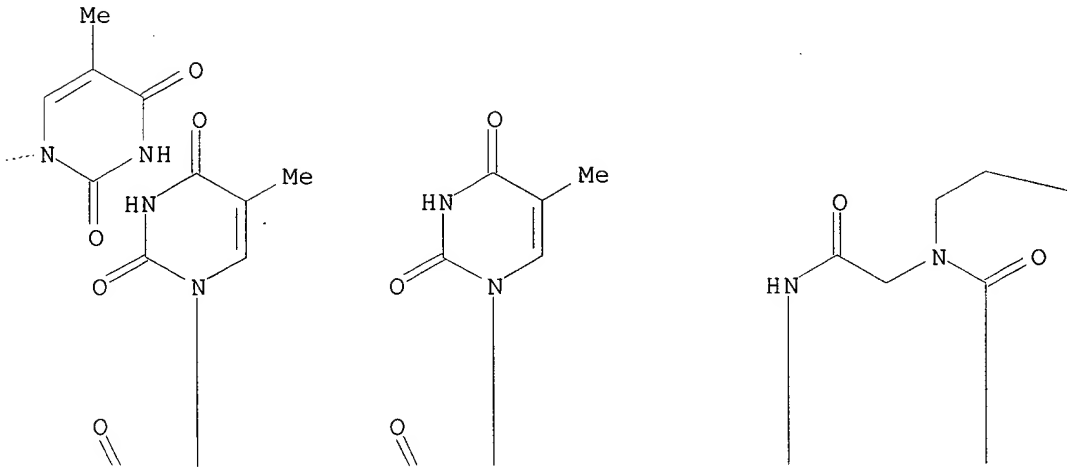
IT **170944-04-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid support synthesis of homothymine peptide nucleic acid-DNA hybrid as antisense oligonucleotide analog)
RN 170944-04-4 HCAPLUS
CN Thymidine, 5'-deoxy-5'-[[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13,19,25-pentaoxo-3,6,9,12,15,18,21,24-octaazahexacos-1-yl]amino]thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



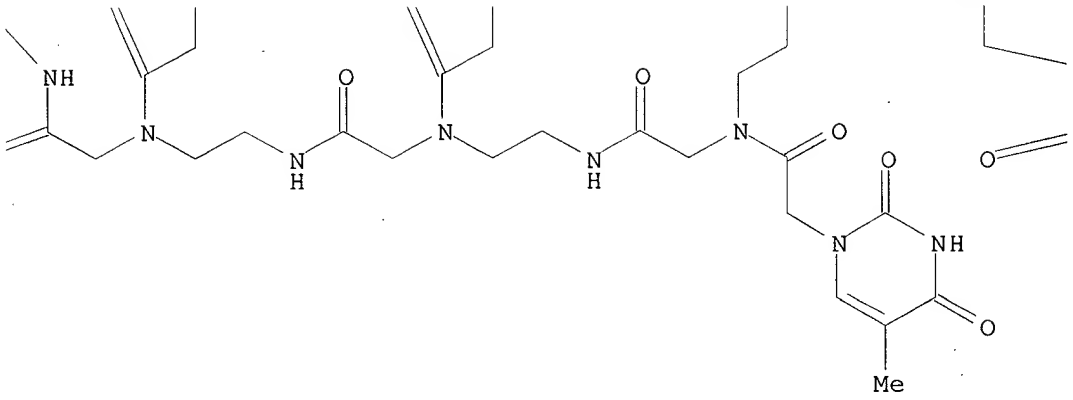
PAGE 1-C

NHAc

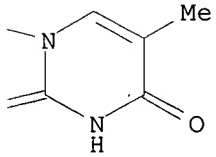
PAGE 2-A

O

PAGE 2-B

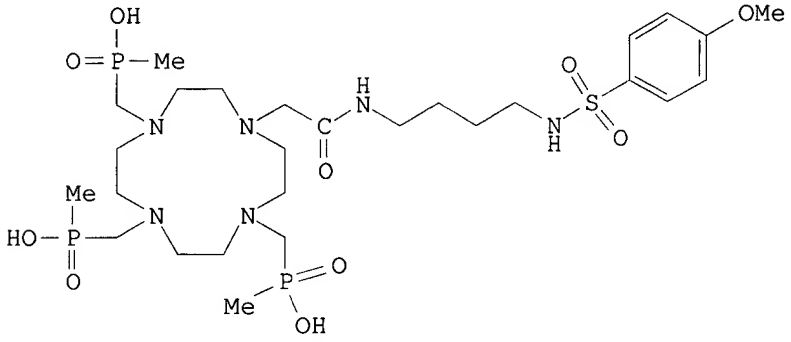


PAGE 2-C



=> d ibib abs hitstr 14

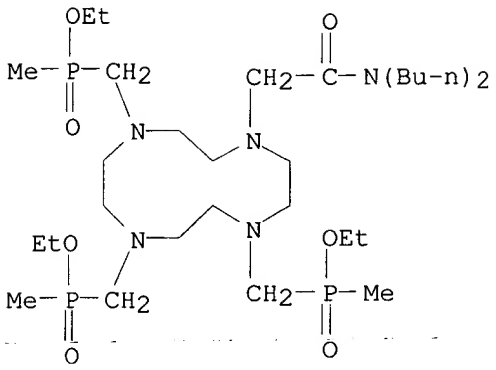
L13 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1994:435685 HCAPLUS
DOCUMENT NUMBER: 121:35685
TITLE: Synthesis of charged and uncharged complexes of gadolinium and yttrium with cyclic polyazaphosphinic acid ligands for in vivo applications
AUTHOR(S): Pulukkody, Kanthi P.; Norman, Timothy J.; Parker, David; Royle, Louise; Broan, Christopher J.
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: J. Chem. Soc., Perkin Trans. 2 (1993), (4), 605-20
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:35685
GI



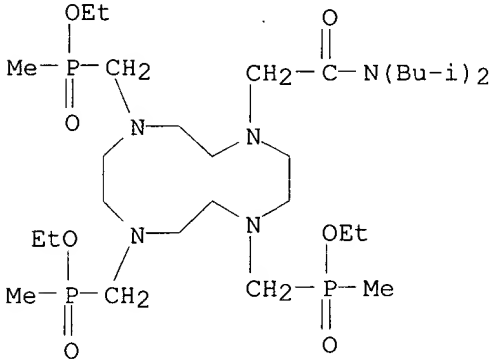
I

AB The synthesis of 18 new macrocyclic complexing agents incorporating phosphinic acid (and carboxylic acid) groups, e.g., I, is reported, based on the 1,4,7,10-tetraazacyclododecane ring. Through selective functionalization of one ring nitrogen or by changing the nature of the P-substituent, anion, neutral and cationic complexes of yttrium and gadolinium may be prepd. of varying lipophilicity. Diamagnetic complexes have been characterized by 1H, 31P and 89Y NMR spectroscopy, and the rate of uptake of 90Y of selected ligands compared. The kinetics of dissocn. of nine gadolinium complexes has been measured in the pH range 1-2 using 153Gd-labeled complexes. Charge-neutral complexes dissoc. more slowly than their anionic analogs, and the phosphinate complexes, although slightly less stable than their carboxylate analogs, are nevertheless sufficiently kinetically inert for in vivo applications.

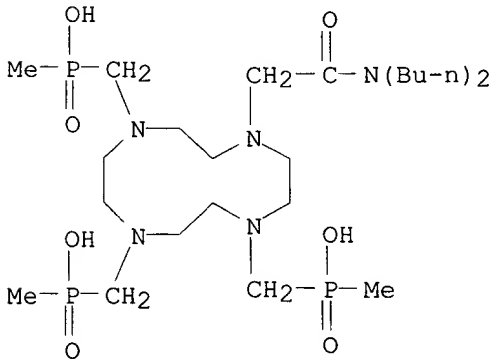
IT **148932-43-8P 148932-55-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and sapon. of)
RN 148932-43-8 HCAPLUS
CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl-, triethyl ester (9CI) (CA INDEX NAME)



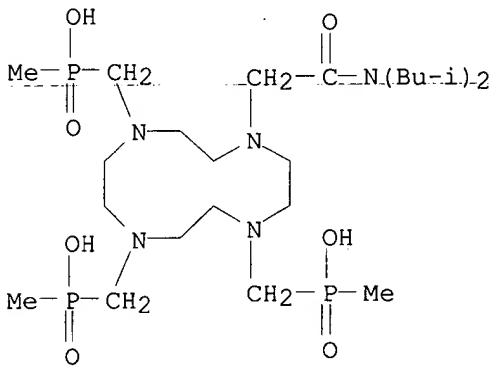
RN 148932-55-2 HCAPLUS
CN Phosphinic acid, [[10-[2-[bis(2-methylpropyl)amino]-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl-, triethyl ester (9CI) (CA INDEX NAME)



IT **145130-40-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and uptake with, of yttrium-90)
RN 145130-40-1 HCAPLUS
CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)



IT **148932-56-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 148932-56-3 HCAPLUS
CN Phosphinic acid, [[10-[2-[bis(2-methylpropyl)amino]-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)

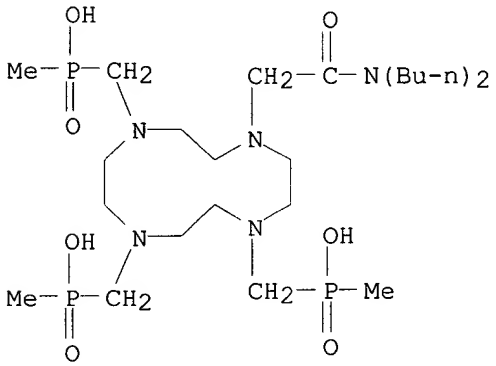


=> d ibib abs hitstr 15

L13 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1993:93170 HCAPLUS
DOCUMENT NUMBER: 118:93170
TITLE: Stable anionic, neutral and cationic complexes of gadolinium with functionalized amino-phosphinic acid macrocyclic ligands
AUTHOR(S): Parker, David; Pulukkody, Kanthi; Norman, Timothy J.; Harrison, Alice; Royle, Louise; Walker, Carol
CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK
SOURCE: J. Chem. Soc., Chem. Commun. (1992), (19), 1441-3
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The synthesis and stability of anionic, neutral and cationic gadolinium complexes based on tetraazaphosphinic acid ligands is compared: lipophilic anionic complexes show biliary rather than renal clearance. The dissocn. kinetics was studied.

IT **145130-40-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and acid hydrolysis and deprotection of)
RN 145130-40-1 HCAPLUS
CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)



IT **145130-40-1DP**, gadolinium and yttrium complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 145130-40-1 HCAPLUS
CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)

4)